09/857, 465

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1204BXD

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | | |
|---|---|---|---|
| NEWS | 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS | 2 | | "Ask CAS" for self-help around the clock |
| NEWS | 3 | FEB 25 | CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered |
| NEWS | 4 | FEB 28 | PATDPAFULL - New display fields provide for legal status data from INPADOC |
| NEWS | 5 | FEB 28 | BABS - Current-awareness alerts (SDIs) available |
| NEWS | 6 | FEB 28 | MEDLINE/LMEDLINE reloaded |
| NEWS | 7 | MAR 02 | GBFULL: New full-text patent database on STN |
| NEWS | 8 | MAR 03 | REGISTRY/ZREGISTRY - Sequence annotations enhanced |
| NEWS | 9 | MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| NEWS | 10 | MAR 22 | KOREAPAT now updated monthly; patent information enhanced |
| NEWS | 11 | MAR 22 | Original IDE display format returns to REGISTRY/ZREGISTRY |
| NEWS | 12 | MAR 22 | PATDPASPC - New patent database available |
| NEWS | 13 | MAR 22 | REGISTRY/ZREGISTRY enhanced with experimental property tags |
| NEWS | 14 | APR 04 | EPFULL enhanced with additional patent information and new fields |
| NEWS | 15 | APR 04 | EMBASE - Database reloaded and enhanced |
| NEWS | 16 | APR 18 | New CAS Information Use Policies available online |
| NEWS | 17 | APR 25 | Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAplus and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications. |
| NEWS | 18 | APR 28 | Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAplus |

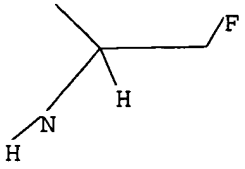
NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

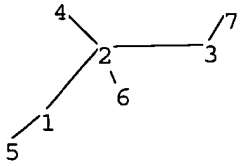
| | |
|---|---|
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

```
  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:40:50 ON 21 MAY 2005

=> fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                             ENTRY    SESSION
FULL ESTIMATED COST                                           0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:40:59 ON 21 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAY 2005  HIGHEST RN 850848-27-0
DICTIONARY FILE UPDATES:  20 MAY 2005  HIGHEST RN 850848-27-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str
```



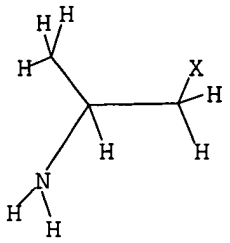




```
chain nodes :
1  2  3  4  5  6  7
chain bonds :
1-2  1-5  2-3  2-4  2-6  3-7
exact/norm bonds :
1-2
exact bonds :
1-5  2-3  2-4  2-6  3-7
```

Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS

L1      STRUCTURE UPLOADED

=> d query
L1              STR




Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:41:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  11760 TO ITERATE

  8.5% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       228703 TO   241697
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:41:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 233651 TO ITERATE

100.0% PROCESSED  233651 ITERATIONS                             15 ANSWERS
SEARCH TIME: 00.00.02

L3           15 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.76     161.97

FILE 'CAPLUS' ENTERED AT 15:41:53 ON 21 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 May 2005 VOL 142 ISS 22
FILE LAST UPDATED: 20 May 2005 (20050520/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 28 L3

=> d l4 1-28 abs ibib hitstr

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

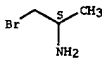
AB New chiral mono- and bicyclic β-sultams, valuable building blocks for drug synthesis, have been prepared from L-Ala, L-Val, L-Leu, L-Ile, L-Phe, L-Cys, L-Ser, L-Thr, and D-penicillamine by transformation of the CO2H group into a methylsulfonyl chloride function, followed by cyclization under basic conditions. Selected properties, derivs., and reactions of the β-sultams are described.

ACCESSION NUMBER: 2004:177034 CAPLUS
DOCUMENT NUMBER: 140:357135
TITLE: Properties and reactions of substituted 1,2-thiazetidine 1,1-dioxides: Chiral mono- and bicyclic 1,2-thiazetidine 1,1-dioxides from α-amino acids
AUTHOR(S): Meinzer, Alexandra; Breckel, Andrea; Thaher, Bassam Abu; Manicone, Nico; Otto, Hans-Hartwig
CORPORATE SOURCE: Department of Pharmaceutical/Medicinal Chemistry, Institute of Pharmacy, University of Greifswald, Greifswald, D-17487, Germany
SOURCE: Helvetica Chimica Acta (2004), 87(1), 90-105
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **53862-15-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral mono- and bicyclic 1,2-thiazetidine 1,1-dioxides from α-amino acids)

RN 53862-15-0 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

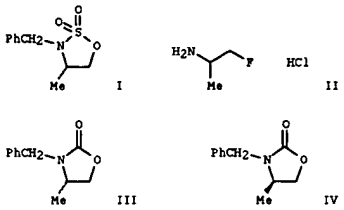


● HBr

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

GI



AB N-benzyl [1,2,3]-oxathiazolidine 2,2-dioxides, e.g. I, (cyclic sulfamidates) were synthesized from their corresponding β-amino alcs. and used as substrates in fluorination reactions with tetrabutylammonium fluoride (TBAF). After desulfonation of the intermediates, the N-benzyl fluoroamines were debenzylated by transfer hydrogenolysis with Pd/C to yield (S) and (R)-2-amino-1-fluoropropane hydrochloride salts (II, both with 95% ee). The reactions were carried out on multi-gram scale without the need for chromatog. purification of the intermediates. In the presence of carbonate, the (S)- and (R)-N-benzylfluoroamines underwent intramol. cyclizations in which fluoride was displaced to yield cyclic carbamates III and IV.

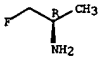
ACCESSION NUMBER: 2002:370219 CAPLUS
DOCUMENT NUMBER: 137:232363
TITLE: Fluoroamines via chiral cyclic sulfamidates
AUTHOR(S): Posakony, Jeffrey J.; Tewson, Timothy J.
CORPORATE SOURCE: Department of Radiology Imaging Research Laboratory, University of Washington, Seattle, WA, 98195, USA
SOURCE: Synthesis (2002), (6), 766-770
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:232363

IT **273734-17-1P 458560-63-9P 459167-94-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluoroamines via chiral cyclic sulfamidates)

RN 273734-17-1 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

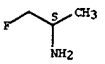
L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



● HCl

RN 458560-63-9 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



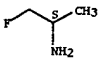
● HCl

RN 459167-94-3 CAPLUS
CN Formic acid, compd. with (2S)-1-fluoro-2-propanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 459167-93-2
CMF C3 H8 F N

Absolute stereochemistry. Rotation (+).



CM 2

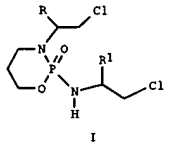
CRN 64-18-6
CMF C H2 O2



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

GI



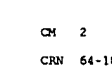
I

AB Three analogs of the cytostatic drug ifosfamide incorporating 1-methyl-2-chloroethyl side chains I (R = H, Me, R1 = Me; R = Me, R1 = H) were designed and prepared as an attempt to obtain drugs of lower toxicity.

ACCESSION NUMBER: 2001:779592 CAPLUS
DOCUMENT NUMBER: 136:85870
TITLE: Synthesis of side-chain-substituted ifosfamide analogs
AUTHOR(S): Paci, Angelo; Guillaume, Dominique; Husson, Henri-Philippe
CORPORATE SOURCE: Laboratoire de Chimie therapeutique, UMR 8638 du CNRS, Faculte des Sciences Pharmaceutiques et Biologiques, Paris, 75006, Fr.
SOURCE: Journal of Heterocyclic Chemistry (2001), 38(5), 1131-1134
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:85870

IT **5968-21-8P**, 1-Methyl-2-chloroethylamine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of chlorooxazaphosphorine oxide with)

RN 5968-21-8 CAPLUS
CN 2-Propanamine, 1-chloro-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB Analogs of arachidonylethanolamide (anandamide) are provided which have higher affinities for the cannabinoid CB1 and/or CB2 receptor sites. Further, most of the analogs exhibit greater metabolic stability than arachidonylethanolamide. The improved receptor affinity and selectivity and/or greater metabolic stability make these analogs therapeutically useful as medications for relief of pain caused by cancer and nausea caused by chemotherapy, as well as for peripheral pain. The compds. may also be useful as oral and topical contraceptives, in suppression of the immune system, enhancement of appetite and in treatment of psychomotor disorders, multiple sclerosis and hypertension.

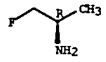
ACCESSION NUMBER: 2000:383939 CAPLUS
DOCUMENT NUMBER: 133:26865
TITLE: Cannabimimetic arachidonylethanolamide (anandamide) derivatives as useful medications, and preparation thereof
INVENTOR(S): Makriyannis, Alexandros; Khanolkar, Atmaram; Goutopoulos, Andreas
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000032200 | A1 | 20000608 | WO 1999-US28136 | 19991124 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1049474 | A1 | 20001108 | EP 1999-961838 | 19991124 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

PRIORITY APPLN. INFO.: US 1998-109615P P 19981124
WO 1999-US28136 W 19991124
OTHER SOURCE(S): MARPAT 133:26865
IT **273734-17-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction; cannabimimetic arachidonylethanolamide derivative preparation for useful medication)
RN 273734-17-1 CAPLUS
CN 2-Propanamine, 1-fluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



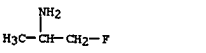
● HCl

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB Conformational geometry changes associated with torsional motion about C-C single bonds are reported for 47 basic organic mols. of the type (XYZ)C-C(X'Y'Z'), and for the .vphi.,.psi. space of model dipeptides (N-acetyl N'-methylamides of glycine and alanine). All structures were determined by ab initio HF/4-21G geometry optimizations. Using natural cubic spline parameters, a program was written for use in empirical modeling-parameter development, which calcs. the bond lengths and angles of the reported compds. as functions of the associated torsional angles at any point in conformational space. The additivity of the conformational-geometry functions is explored, and illustrates how cooperative effects emerge in complex mols. The results are instructive for procedures in which the properties of mol. fragments are used to derive force-field parameters for the empirical modeling of complex mols.

ACCESSION NUMBER: 1997:666340 CAPLUS
DOCUMENT NUMBER: 127:346003
TITLE: Conformational geometry functions: additivity and cooperative effects
AUTHOR(S): Schaefer, Lothar; Cao, Ming; Ramek, Michael; Teppen, Brian J.; Newton, Susan Q.; Siam, Khamis
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR, USA
SOURCE: Journal of Molecular Structure (1997), 413-414, 175-204
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **66679-45-6**, 2-Propanamine, 1-fluoro-
RL: PRP (Properties)
(additivity and cooperative effects in conformational geometry functions for small org mols. by HF MO)
RN 66679-45-6 CAPLUS
CN 2-Propanamine, 1-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB Title compds. H2NCHRCHR1SC(:NH)NH2.2HBr [R = H, Me, Pr; R1 = H, Me], which possess antiactinic activity, are prepared by reaction of H2NCHRCHR1Br.HBr with thiourea in an anhydrous organic solvent under heating, with isolation of product by repeated recrystn. from 1:1 EtOAc/EtOH mixture, and repeated boiling in anhydrous Me2CO. In particular, the anhydrous organic reaction solvent is specified as a 5:1.2 EtOAc/EtOH mixture

ACCESSION NUMBER: 1995:995131 CAPLUS
DOCUMENT NUMBER: 124:86380
TITLE: Dihydrobromides of S-(2-aminoalkyl)- or S-(1-amino-2-propyl)isothioureas possessing antiactinic activity and method of their preparation
INVENTOR(S): Mandrugin, A. A.; Fedoseev, V. M.; Tarasenko, A. G.; Nekrasova, I. V.; Gintsburg, E. P.
PATENT ASSIGNEE(S): MGU im.M.V.Lomonosova, Russia
SOURCE: U.S.S.R. From: Izobreteniya 1995, (4), 241.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

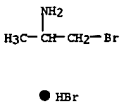
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| SU 577785 | A1 | 19950209 | SU 1975-2115876 | 19750319 |

PRIORITY APPLN. INFO.: SU 1975-2115876 19750319
OTHER SOURCE(S): CASREACT 124:86380
IT **2403-31-8**, 2-Amino-1-bromopropane hydrobromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of S-aminoalkyl and S-aminopropyl isothiourea dihydrobromides with antiactinic activity)
RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)



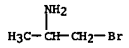
● HBr

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB Reaction of 2-chloropropylamine hydrochloride (I) with 10% pyrrolidine (NR2H) in benzene in presence of K2CO3 afforded NH2CHMeCH2NR2 + NH2CH2CHMeNR2 in ratio of 1:3, resp. Since the analogous reaction of 2-amino-1-bromopropane hydrobromide afforded exclusively NH2CHMeCH2NR2, the formation of NH2CH2CHMeNR2 reflects direct nucleophilic substitution on substrate I. Mixing is of extreme importance, as it prevents accumulation of dissolved ammonium salt leading to structures NH2CHMeCH2NR2.
ACCESSION NUMBER: 1995:400781 CAPLUS
DOCUMENT NUMBER: 122:290797
TITLE: Direct nucleophilic substitution on 2-haloalkylamines: a novel method to synthesize substituted ethylenediamines
AUTHOR(S): Chechik, V. O.; Bobylev, V. A.
CORPORATE SOURCE: Ross. Nauchn. Tsentr. "Prikadnaya Khimiya", St. Petersburg, Russia
SOURCE: Zhurnal Obshchei Khimii (1994), 64(10), 1685-7
CODEN: ZOKHA4; ISSN: 0044-460X
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 122:290797
IT 2403-31-8, 2-Amino-1-bromopropane hydrobromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted ethylenediamines via direct nucleophilic substitution reaction on 2-haloalkylamines:)
RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)

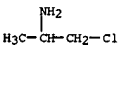


● HBr

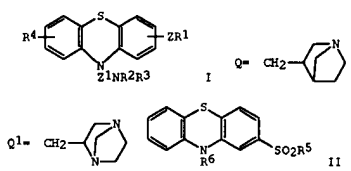
L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB The kinetics of cyclization of 5-halopentylamines in DMSO-water mixts. have been studied and compared with previously reported data on the cyclization of 2-haloethylamines. The results prove the transition state of the latter reaction to be later and consequently more polar. Specifically solvating and polar solvents would therefore favor the formation of 3-membered rings as compared to unstrained medium-sized ones. This conclusion makes it possible to determine the conditions under which direct nucleophilic substitution on 2-haloalkylamines does successfully compete with the intramol. formation of aziridines.
ACCESSION NUMBER: 1994:533363 CAPLUS
DOCUMENT NUMBER: 121:133363
TITLE: Competition between three-membered-ring formation and intermolecular substitution: solvent effect
AUTHOR(S): Chechik, Victor O.; Bobylev, Vladimir A.
CORPORATE SOURCE: Russian Sci. Cent. "Prikladnaja Khimija", St. Petersburg, 197198, Russia
SOURCE: Journal of Chemical Research, Synopses (1994), (7), 256-7
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 72696-68-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with cyclic amines, solvent effect on)
RN 72696-68-5 CAPLUS
CN 2-Propanamine, 1-bromo- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB A kinetic study of the cyclization of MeCHClCH2NH2 and MeCH(NH2)CH2Cl to 2-methylaziridine in aqueous NaOH or aqueous ethylenediamine indicated an A2 mechanism with a late transition state. The lower cyclization ability of Cl(CH2)3NH2 resulted from an entropic factor.
ACCESSION NUMBER: 1990:514451 CAPLUS
DOCUMENT NUMBER: 113:114451
TITLE: Study of the kinetics and mechanism of cyclization of chloropropylamines
AUTHOR(S): Chernitskii, K. V.; Bobylev, V. A.; Veselkov, N. Yu.
CORPORATE SOURCE: Gos. Inst. Prikl. Khim., Leningrad, USSR
SOURCE: Zhurnal Obshchei Khimii (1990), 60(3), 625-32
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT 37143-56-9, 2-Amino-1-chloropropane
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(cyclization of, kinetics of)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
GI

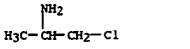


AB The title compds. [I; R1 = an acidic group other than a monocarboxylic acid group, having acidity ≥CO2H; R2,R3 = H, alkyl; R2R3N = heterocyclyl; R4 = H, (halo)alkyl, alkoxy, halo, HO2CZ; Z = bivalent, aliphatic hydrocarbon group, bond; Z1 = alkylene; R2R3NZ1 = Q, Q1] and their esters and amides were prepared Thus, 4,3-Cl(O2N)C6H3SO2NMe2 and 2-BrC6H4SNa were refluxed in ethanolic NaOH to give 95% 2-BrC6H4SC6H4(NO2)SO2NMe2-2,4 which was reduced to the amine (84%) with Fe powder in EtOH/HOAc. The latter was cyclized by refluxing with Cu bronze and K2CO3 in DMF to give phenothiazinesulfonamide II (R5 = Me2N, R6 = H). This was alkylated with Me2N(CH2)3Cl and deamidated by heating with Na in Me2CHCH2CH2OH to give II [R5 = OH, R6 = Me2N(CH2)3] (III). III is a histamine receptor antagonist with pA2 = 7.8 in the isolated guinea pig ileum test.
ACCESSION NUMBER: 1986:148893 CAPLUS
DOCUMENT NUMBER: 104:148893
TITLE: Phenothiazine compounds
INVENTOR(S): Leighton, Harry Jefferson; Gillies, Iain
PATENT ASSIGNEE(S): Wellcome Foundation Ltd., UK
SOURCE: Eur. Pat. Appl., 43 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 163551 | A1 | 19851204 | EP 1985-303875 | 19850531 |
| EP 163551 | B1 | 19920812 | | |
| R: CH, DE, FR, GB, IT, LI | | | | |
| SU 1731052 | A3 | 19920430 | SU 1984-3829883 | 19841227 |
| US 4705854 | A | 19871110 | US 1985-738846 | 19850528 |
| JP 61044884 | A2 | 19860304 | JP 1985-118690 | 19850531 |
| PRIORITY APPLN. INFO.: | | | GB 1984-13915 A | 19840531 |

IT 37143-56-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of phenothiazines)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



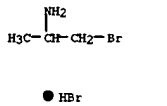
L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB The title compound (I) was prepared from Me3CCOCl and NaO2CH in the presence of 18-crown-6. I was a very useful reagent for the N-formylation of amines. Even amines which are unstable when deprotonated can be formylated.

ACCESSION NUMBER: 1983:88790 CAPLUS
DOCUMENT NUMBER: 98:88790
TITLE: Trimethylacetic formic anhydride. Improved preparation and use as a highly efficient and selective N-formylating reagent
AUTHOR(S): Vlietstra, Edward J.; Zwikker, Jan W.; Nolte, Roeland J. M.; Drenth, Wiendelt
CORPORATE SOURCE: Lab. Org. Chem., Univ. Utrecht, Utrecht, 3522 AD, Neth.
SOURCE: Recueil: Journal of the Royal Netherlands Chemical Society (1982), 101(12), 460-2
CODEN: RJRSDK; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:88790

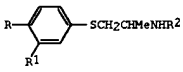
IT **2403-31-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(formylation of, with pivalic formic anhydride)

RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)



L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

GI



I

AB Title compds. I (R = halo; R1 = H, halo; R2 = Me, Et, CH2CH2OH) were prepared and found to have antiobesity and antidiabetic activity. E.g., reaction of 4-ClC6H4SH with ClCH2COMe gave 4-ClC6H4SCH2COMe, which was treated with MeNH2, MeNH2.HCl and NaBH3CN in MeOH to give 1-(4-chlorophenylthio)-2-(methylamino)propane fumarate. Alternatively, N-carbobenzyloxy-L-alanine was reduced with LiAlH4 to S-2-(methylamino)propanol, then treated with SOCl2 followed by 4-ClC6H4SH to give (S)-1-(4-chlorophenylthio)-2-methylaminopropane, isolated as the fumarate.

ACCESSION NUMBER: 1982:562565 CAPLUS
DOCUMENT NUMBER: 97:162565
TITLE: 1-(Phenylthio)-2-aminopropane derivatives and their use
INVENTOR(S): Meguro, Kanji; Matsuo, Takao
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd. , Japan
SOURCE: Eur. Pat. Appl., 40 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

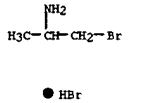
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 53015 | A1 | 19820602 | EP 1981-305495 | 19811120 |
| R: CH, DE, FR, GB, IT | | | | |
| JP 57088162 | A2 | 19820601 | JP 1980-164862 | 19801121 |
| JP 58004760 | A2 | 19830111 | JP 1981-101454 | 19810629 |
| DK 8201010 | A | 19821230 | DK 1982-1010 | 19820309 |
| SE 8201618 | A | 19821230 | SE 1982-1618 | 19820315 |
| PRIORITY APPLN. INFO.: | | | JP 1980-164862 A | 19801121 |
| | | | JP 1981-101454 A | 19810629 |

OTHER SOURCE(S): CASREACT 97:162565

IT **2403-31-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with chlorothiophenol)

RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)

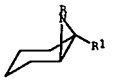
L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB D- and 18O-labeling studies indicated that ClCH2CHRNHCON(NO)CHRCH2Cl (I, R = H) decomposed in phosphate buffer (pH 7.1) in the presence of liver alc. dehydrogenase and NADH with a 21% contribution from the path via a 1,2,3-oxadiazoline intermediate. This intermediate may decompose partly by a concerted path involving a D shift. In contrast, the 1,2,3-oxadiazoline path contributed 89% to the analogous decomposition of I (R = Me). A possible reason for these results was discussed.

ACCESSION NUMBER: 1982:84902 CAPLUS
DOCUMENT NUMBER: 96:84902
TITLE: Discrimination between alternative pathways of aqueous decomposition of antitumor (2-chloroethyl)nitrosoureas using specific oxygen-18 labeling
AUTHOR(S): Lown, J. William; Chauhan, Shive M. S.
CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Journal of Organic Chemistry (1982), 47(5), 851-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:84902
IT 80326-82-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phosgene)
RN 80326-82-5 CAPLUS
CN 2-Propan-1,1-d2-amine, 1-chloro- (9CI) (CA INDEX NAME)

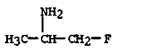
L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB Ring-opening of secondary aziridines with anhydrous HF or Olah's reagent, and of N-activated aziridines by NEt3-nHF (n = 2, 2.5, 3) provides an efficient synthetic route to α,β-fluoroamines. The stereochem. of the reaction appears to be very dependent on the structure of the aziridine and on the fluorinating reagent. Thus in acyclic series, secondary aziridines can react with anhydrous HF with inversion of configuration, whereas Olah's reagent always leads to a carbocation formation which is then quenched by a fluoride ion delivered by the ammonium group. With bicyclic aziridines I (R = H, R1 = Ph, Et, H) this latter reaction yields cis-fluoroamines. In contrast, when N-carbo-tert-butoxy aziridines are treated with partially neutralized Olah's reagent (NEt3-nHF) exclusive inversion of configuration is observed in acyclic or cyclic series, leading from compds. I (R = CO2CMe3, R1 = Ph, Et, H) only to trans-fluoroamines. It is thus possible by proper choice of the fluorination method to direct the stereochem. of the final fluoroamine.

ACCESSION NUMBER: 1981:603644 CAPLUS
DOCUMENT NUMBER: 95:203644
TITLE: Ring opening of aziridines by different fluorinating reagents: three synthetic routes to α,β-fluoro amines with different stereochemical pathways
AUTHOR(S): Alvernhe, Gerard M.; Ennakoua, Christine M.; Lacombe, Sylvie M.; Laurent, Andre J.
CORPORATE SOURCE: Lab. Chim. Org. III, Univ. Claude Bernard, Villeurbanne, 69622, Fr.
SOURCE: Journal of Organic Chemistry (1981), 46(24), 4938-48
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:203644
IT 66679-45-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66679-45-6 CAPLUS
CN 2-Propanamine, 1-fluoro- (9CI) (CA INDEX NAME)

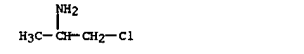


L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB Eight insecticidal title compds., XCH2CHFOP(O)(R)NR1CR3R4CR5R6SR2 (I, R = alkyl, alkoxy, R1 = H, alkyl, R2 = Me, Et, Pr, Me2CH, R3-6 = H, Me, Et, X = Cl, Br) were prepared by esterification and amidation of XCH2CHFOP(O)Cl2 (II). Thus, 0.1 mol II (X = Cl), 0.1 mol EtOH, 0.1 mol MeSCH2CH(NH2)Me, and 0.2 mol Et3N in PhMe gave 95.6% ClCH2CHFOP(O)(OEt)NHCHMeCH2SMe.

ACCESSION NUMBER: 1981:102857 CAPLUS
DOCUMENT NUMBER: 94:102857
TITLE: O-(1-Fluoro-2-haloethyl) phosphoric(phosphonic) acid ester amides
INVENTOR(S): Arlt, Dieter; Homeyer, Bernhard
PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

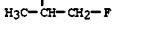
| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|---|---|---|---|---|---|
| DE 2904927 | A1 | 19800821 | DE 1979-2904927 | | 19790209 |
| PRIORITY APPLN. INFO.: | | | DE 1979-2904927 | A | 19790209 |

IT 37143-56-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with sodium methylmercaptide)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)

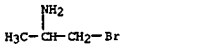


L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB The dissociation consts. were determined for 12 α-fluorinated amines in aqueous 2-methoxyethanol. The α-fluorinated amines were of the general formula R1-CHF-CHR2-N(R3R4) where R1 = H, alkyl or Ph group and R2 = H or alkyl group.

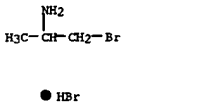
ACCESSION NUMBER: 1980:413965 CAPLUS
DOCUMENT NUMBER: 93:13965
TITLE: Determination of the dissociation constants of a series of α-fluorinated amines in mixtures of water and 2-methoxyethanol
AUTHOR(S): Abdelkafi, Mohamed Mouldi; Baklouti, Ahmed
CORPORATE SOURCE: Fac. Sci., Campus Univ. Tunis, Tunis, Tunisia
SOURCE: Journal de la Societe Chimique de Tunisie (1979), (1), 1-15
CODEN: JSCTDP; ISSN: 0253-1208
DOCUMENT TYPE: Journal
LANGUAGE: French
IT 66679-45-6
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(ionization of, in aqueous methoxyethanol)
RN 66679-45-6 CAPLUS
CN 2-Propanamine, 1-fluoro- (9CI) (CA INDEX NAME)



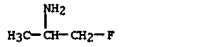
L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB Preparation of aminoalkylphosphonic acids by amino group protection by nitrogen-phosphorus bond formation is reported. Phosphorylation of β- or γ-bromoalkylamines with chlorophosphates followed by Arbuzov reaction with (EtO)3P gave a phosphoramidate-phosphonate intermediate which was alkylated by various reagents. The phosphoryl residue was removed by treatment with aqueous HCl.
ACCESSION NUMBER: 1980:76599 CAPLUS
DOCUMENT NUMBER: 92:76599
TITLE: Preparation of aminoalkylphosphonic acids with the help of phosphorylated ω-haloalkyl amines
AUTHOR(S): Brigot, D.; Collignon, N.; Savignac, P.
CORPORATE SOURCE: Lab. Chim. Org., Inst. Natl. Super. Chim. Ind. Rouen, Mont-Saint-Aignan, 76130, Fr.
SOURCE: Tetrahedron (1979), 35(11), 1345-55
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 92:76599
IT **72696-68-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with di-Et chlorophosphate)
RN 72696-68-5 CAPLUS
CN 2-Propanamine, 1-bromo- (9CI) (CA INDEX NAME)



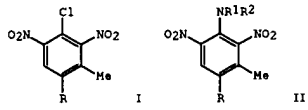
L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB The kinetics of the hydrolysis of bromoethylamine-HBr derivs. (e.g., BrCH2CH2NH3+ Br-, BrCH2CHMeNH3+ Br-, MeCHBrCH2NH3+ Br-, Me2CBrCHMeNH3+ Br-), determined at 80-100° under conditions in which the free amine was absent, exhibited an isokinetic relation with β 94 ± 10°.
ACCESSION NUMBER: 1978:507631 CAPLUS
DOCUMENT NUMBER: 89:107631
TITLE: Acid hydrolysis of 2-haloethylamines. II. Measurements in the 80-100° temperature range. Demonstration of an isokinetic relation
AUTHOR(S): Lamaty, G.; Sivade, A.
CORPORATE SOURCE: Lab. Chim. Org. Phys., Univ. Sci. Tech. Languedoc, Montpellier, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1974), (9-10, Pt. 2), 2149-53
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **2403-31-8**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(hydrolysis of, kinetics of)
RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)



L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB The apparent pK of 16 RCHFCHR1NR2R3 [R = H, Me, Et, Bu, Ph; R1 = H, Me (threo and erythro), Et; R2, R3 = H or alkyl] were determined by potentiometric titration in MeOCH2CH2OH-H2O. Substituent effects were discussed, e.g., the α-F decreases the basicity of the amine.
ACCESSION NUMBER: 1978:405760 CAPLUS
DOCUMENT NUMBER: 89:5760
TITLE: Determination of the dissociation constants of an α-fluorinated amines series in a water/2-methoxyethanol mixture
AUTHOR(S): Abdelkafi, Mohamed Mouldi; Baklouti, Ahmed
CORPORATE SOURCE: Lab. Chim. Org. Struct., Fac. Sci. Tunis, Tunis, Tunisia
SOURCE: Bulletin de la Societe Chimique de France (1977), (11-12, Pt. 1), 1044-8
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
IT **66679-45-6**
RL: PRP (Properties)
(dissociation constant of, in methoxyethanol-water)
RN 66679-45-6 CAPLUS
CN 2-Propanamine, 1-fluoro- (9CI) (CA INDEX NAME)



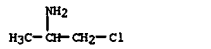
L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB The substitution reaction of chlorodinitrobenzenes I (R = Me, Cl, SO2NH2, substituted sulfamoyl, CF3, CN) with amines gave seventy-eight anilines II (R1 = H, C1-4 alkyl, allyl; R2 = H, C1-7 alkyl, allyl, alkoxyalkyl, chloroalkyl, Ph; NR1R2 = piperidino, morpholino, pyrrolidinyl), most of which exhibited herbicidal activity.
ACCESSION NUMBER: 1977:467960 CAPLUS
DOCUMENT NUMBER: 87:67960
TITLE: 2,6-Dinitroaniline herbicides
INVENTOR(S): Lutz, Albert William; Diehl, Robert Eugene
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 17 pp. Division of U.S. 3,920,742.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 9
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 4025538 | A | 19770524 | US 1975-599224 | 19750725 |
| US 3920742 | A | 19751118 | US 1973-323000 | 19730112 |
| IN 147315 | A | 19800126 | IN 1978-CA852 | 19780804 |
| PRIORITY APPLN. INFO.: | | | US 1971-174938 | A2 19710825 |
| | | | US 1972-262807 | A2 19720614 |
| | | | US 1973-323000 | A3 19730112 |
| | | | US 1975-642806 | A 19751222 |
| | | | IN 1976-CA2170 | A1 19761208 |

IT **37143-56-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with chlorodinitrobenzenes)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)



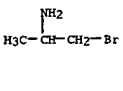
L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB Rate consts. and activation parameters were determined for the hydrolysis in 0.1 N HClO4 of BrCRR1CR2R3NH2.HBr (R, R1, R2 = H or Me, R3 = H, Me, or Et) at 50, 60, 70, 80, 90, and 100°. An isokinetic relation, with isokinetic temperature 94±10°, was observed and the study showed the absence of a neopentylic retardation effect when R = R1 = H and R2 = R3 = Me and showed a modest increase of reactivity when R = R1 = Me. The results are discussed on the basis of an electrostatic intramol. interaction mechanism.

ACCESSION NUMBER: 1976:89080 CAPLUS
DOCUMENT NUMBER: 84:89080
TITLE: Acidic hydrolysis of 2-haloethylamines. III. Kinetic measurements in the 50-80.deg. temperature range. Comparative analysis of the results at 50.deg. as a function of the structural variation of the substrate
AUTHOR(S): Lamaty, Gerard; Sivade, Andre
CORPORATE SOURCE: Lab. Chim. Org. Phys., Univ. Sci. Tech. Languedoc, Montpellier, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1975), (7-8, Pt. 2), 1828-36
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

IT **2403-31-8**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(hydrolysis of, kinetics of)

RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)



● HBr

L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

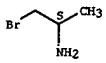
AB Poly(S-2-aminoethyl-L-cysteine) (I), poly(S-3-aminopropyl-L-cysteine) (II), poly(S-L-2-aminopropyl-L-cysteine) (III), and poly(S-D-2-aminopropyl-L-cysteine) (IV) were prepared by the N-carboxyanhydride method via the benzyloxycarbonyl derivs. of the amino polymers. The β-coil transition of the protected polymers occurred at 3-15% dicyclohexylamine in CHCl3. At pH 3-8 in aqueous solution, I-IV are in a random coil, and at .apprx.pH 9 change to the β-conformation.

ACCESSION NUMBER: 1974:569809 CAPLUS
DOCUMENT NUMBER: 81:169809
TITLE: Syntheses and conformational studies of poly(S-aminoalkyl-L-cysteines) and their benzyloxycarbonyl derivatives
AUTHOR(S): Hayakawa, Tadao; Kondo, Yoshiyuki; Murakami, Yukiko
CORPORATE SOURCE: Fac. Text. Sci. Technol., Shinshu Univ., Ueda, Japan
SOURCE: Polymer Journal (Tokyo, Japan) (1974), 6(5), 424-30
CODEN: POLJB8; ISSN: 0032-3896
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **53862-15-0P 53862-16-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with benzyloxycarbonyl halide)

RN 53862-15-0 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide, (2S)- (9CI) (CA INDEX NAME)

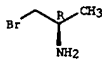
Absolute stereochemistry.



● HBr

RN 53862-16-1 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HBr

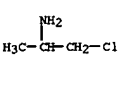
L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB 3-Methylpyrrolidine [34375-89-8] and sec-butylamine [13952-84-6] were the most active of 50 nonaromatic amines tested in their cationic form for inhibition of germination of Penicillium digitatum spores. Pyrrolidine [123-75-1], 2-methylpyrrolidine [765-38-8], isopropylamine [75-31-0], 1-methyl-2-propenylamine [34375-90-1], and cyclobutylamine [2516-34-9], showed lesser activity, but all other simple amines tested were not inhibitory. Replacement of the C-1 or C-4 methyl group of sec-butylamine with CF3, CCl3, CO2H, OMe, CH2OH, Cl, NH2, or OH resulted in compds. which were not active. (-)-Sec-butylamine [13250-12-9] was considerably more active than (+)-sec-butylamine [513-49-5], both in preventing spore germination, and in inhibiting mycelial growth of three species of fungi which were sensitive to racemic sec-butylamine. (-)-Sec-butylamine and 3-methylpyrrolidine were uniquely effective in preventing infection of stored citrus fruits by P. digitatum. The receptor site for inhibitory amines on the fungus cell appears to consist of an anionic component which binds the NH3+ group and a hydrophobic area which is complementary to the sec-butyl radical as spatially oriented in (-)-sec-butylamine.

ACCESSION NUMBER: 1972:430124 CAPLUS
DOCUMENT NUMBER: 77:30124
TITLE: Fungistatic activity of cations of nonaromatic amines
AUTHOR(S): Eckert, Joseph W.; Rahm, Michael L.; Kolbezen, Martin J.
CORPORATE SOURCE: Dep. Plant Pathol., Univ. California, Riverside, CA, USA
SOURCE: Journal of Agricultural and Food Chemistry (1972), 20(1), 104-9
CODEN: JAFCAU; ISSN: 0021-8561
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **37143-56-9**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(fungicidal activity of)

RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

AB To chlorinate saturated amines in other than the α-position, Cl is passed through a solution of the amine in a strong acid, with light or azobis(isobutyronitrile) (I) as catalyst, at 75-120°. Thus, to a solution of 11.25 g. EtNH2 in 22 g. concentrated H2SO4 and 22 g. 20% oleum (II) Cl is added 5 hrs. at 80-5°, while a total of 1 g. I is added in 30 portions to give ClCH2CH2NH2.HCl, m. 135°. In the same manner are prepared from the corresponding saturated amines (product, m.p. or b.p., solvent, catalyst, reaction temperature, and time are given): Cl2CHCH2NH2, b20 32°, II, 450-w. high pressure mercury arc-lamp (III), 50° 90 min.; Cl3CCH2NH2, b20 42-3°, II, III, 50°, 3 hrs.; ClCH2CH2NEt2, b22 54-6°, II, I, 90-100°, 2 hrs.; Cl2CHCH2NMe2, b53 65-66°, II, I, 80-85°, 4 hrs.; ClCH2CHMeNH2, --, II, III, 70°, 1 hr.; Cl2CHCHMeNH2.HCl, m. 187°, ClSO3H, III, 55-60° 90 min.; (Cl2CH)2CHNH2, --, II, --, 60-5°, 3 hrs.; (Cl3C)2CHNH2, --, II, --, 60-5°, 6 hrs.; 4-chloropiperidine, --, FSO3H, uv light, 40-5°, 50 min.; (ClCH2CH2)3N, b2 98°, II, uv light, 60-5°, 2.5 hrs.; 4-chloroquinuclidine, --, F3CCOOH, uv light, 35-40°, 1 hr.

ACCESSION NUMBER: 1966:59476 CAPLUS
DOCUMENT NUMBER: 64:59476
ORIGINAL REFERENCE NO.: 64:11084b-d
TITLE: Chlorination of saturated amines
PATENT ASSIGNEE(S): Merck & Co., Inc.
SOURCE: 11 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| NL 6505505 | | 19651105 | NL | |
| | | | US | 19640504 |

PRIORITY APPLN. INFO.:

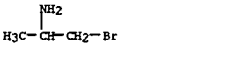
IT **5968-21-8**, Ethylamine, 2-chloro-1-methyl-, hydrochloride
(preparation of)

RN 5968-21-8 CAPLUS
CN 2-Propanamine, 1-chloro-, hydrochloride (9CI) (CA INDEX NAME)

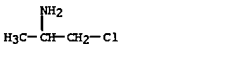


● HCl

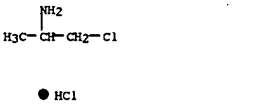
L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB In the reaction of 2-amino-1-bromopropane hydrobromide with 1 equivalent of sodium thiosulfate, the formation of only one product, 2-aminopropane-1-thiosulfuric acid (I), is detected. Similar treatment of 1-amino-2-bromopropane hydrobromide (II) yields two products, namely, 1-aminopropane-2-thiosulfuric acid (III) and the rearranged product I. In order to determine whether an ethylenimonium ion is an intermediate in the formation of I in the latter reaction, the ring opening of 2-methylethylenimine by thiosulfate ion was investigated. The direct displacement of bromide in II by thiosulfate ion without the intermediacy of the cyclic imonium ion accounts for the formation of III. The ratio of the rate constants for the intramolecular displacement vs. the intermolecular displacement was found to be 1.45.
ACCESSION NUMBER: 1965:430997 CAPLUS
DOCUMENT NUMBER: 63:30997
ORIGINAL REFERENCE NO.: 63:5468h,5469a-b
TITLE: Nucleophilic displacement of bromide by thiosulfate ion from 1,2-aminobromopropanes
AUTHOR(S): Klayman, Daniel L.; Lown, James W.; Sweeney, Thomas R.
CORPORATE SOURCE: Walter Reed Army Inst. of Res., Washington, DC
SOURCE: Journal of Organic Chemistry (1965), 30(7), 2275-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 2403-31-8, Ethylamine, 2-bromo-1-methyl-, hydrobromide
(reaction with Na2S2O3, kinetics of)
RN 2403-31-8 CAPLUS
CN 2-Propanamine, 1-bromo-, hydrobromide (9CI) (CA INDEX NAME)



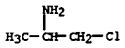
L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB Fibrous ion-exchange derivs. of cellulose were prepared by 2 etherification processes: (1) the reaction of chloroalkylamines and alkali cellulose and (2) the reaction of aminoalkyl H sulfates with alkali cellulose. Side reactions between the reagent and excess alkali in the reaction mixture resulted in low (30% based on the aminoalkylating agent) yields of the cellulose derivs. Thus, 10 g. of purified wood cellulose was homogenized in the cold with 40 g. 5N NaOH. The cellulose was then reacted with an aqueous solution of 12 g. of 2-chloroethyldibutylamine hydrochloride at 95° for 100 min. After washing with HCl and NaOH solns., the product was washed free of salts. Similarly, cellulose derivs. were prepared from chloroethylamine, chloroisopropylamine, chlorodimethylamine, chlorodiethylamine, chloroethyl diisopropylamine, chloroethyldibutylamine and the following aminoalkyl hydrogen sulfates: aminoethyl, dimethylaminoethyl, diethylaminoethyl, diisopropylaminoethyl, dibutylaminoethyl, and bis-2-(ethylhexyl)aminoethyl. Anion-exchange capacities of up to 2 meq./g. of dry cellulose derivs. were obtained. Equilibrium swelling with H2O varied from 55 to 80%. The ion exchangers were
stable in solns. of pH 0-14 and unaffected by mild oxidants such as dilute aqueous chlorate and dichromate solns.
ACCESSION NUMBER: 1961:107658 CAPLUS
DOCUMENT NUMBER: 55:107658
ORIGINAL REFERENCE NO.: 55:20260i,20261a-c
TITLE: Anion exchangers based on cellulose. I. Preparation and general properties
AUTHOR(S): Jakubovic, A. O.; Brook, B. N.
CORPORATE SOURCE: W. & R. Balston Ltd., Maidstone, UK
SOURCE: Polymer (1961), 2, 18-26
CODEN: POLMAG; ISSN: 0032-3861
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 37143-56-9, Ethylamine, 2-chloro-1-methyl-
(reaction product with cellulose, anion-exchanging)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)



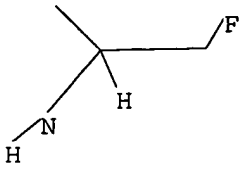
L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB D- or L-Propylenimine (I), b. 67°, [α]21D 12.4° and -12.8° (c 2, EtOH), were prepared from alaninol (II) via either the sulfate ester or the chloride HCl salt, followed by NaOH cyclization. II, prepared by LiAlH4 reduction of D-or L-MeCH(NH2)CO2Et, b23 84° and b26 91°, n29D 1.4493-5, [α]25D 21.8° (c 2.94, EtOH) or -21.8° (c 2.75). H2SO4 (50% by volume) added slowly to II gave 90% dl-2-aminopropylsulfuric acid (III), m. 231°, L-isomer, m. 246°, and D-isomer, m. 247°. III mixed with aqueous NaOH and distilled gave 60% D- and L- I, m. -44°, n27.5D 1.4156. II in 36% HCl gave the salt which after H2O removal and treatment in CHCl3-SOCl2 gave 83% β-chloroisopropylamine-HCl which with alkali gave 19% I. 1-Methylamino-2-propanol (IV), m. 17°, b26 73-4°, was prepared in 66% yield from aqueous MeNH2 with 1,2-propylene oxide at -5 to 5°. IV heated to the char point with 98% H2SO4, cooled, treated with 40% aqueous NaOH, and distilled gave 30-35% N-methylpropylenimine (V), b. 42-3°. Alanine Et ester with MeI in the presence of alc. and K2CO3 gave 20% N-Me derivative, b60 78-80°, and this on LiAlH4 reduction gave 45% N-Me derivative
of II, b23 48-51°, which cyclized with SOCl2 to the chloride HCl salt then treated with aqueous 40% NaOH also gave 20% V. IR spectra of the imines were given. I was polymerized with HCl, BF3, p-MeC6H4SO3H, and other catalysts. The racemic monomer gave an oily polymer while the optically active ones gave solid optically active polymers of low mol. weight, soluble in
MeOH, EtOH, and H2O, but insol. in Et2O, Me2CO, C6H6, and dioxane. Intrinsic viscosities, softening points, and [α]D of a number of polymers were given. V gave a polymer of mol. weight 2000-4000 with FeCl3 catalyst. Imine polymns. were carried out at 80° and required a number of days.
ACCESSION NUMBER: 1960:44578 CAPLUS
DOCUMENT NUMBER: 54:44578
ORIGINAL REFERENCE NO.: 54:8772d-h
TITLE: Preparation and polymerization of D- and L-propylenimine and N-methylpropylenimine
AUTHOR(S): Minoura, Yuji; Takebayashi, Matsuji; Price, Charles C.
CORPORATE SOURCE: Univ. of Pennsylvania, Philadelphia
SOURCE: Journal of the American Chemical Society (1959), 81, 4689-92
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:44578
IT 5968-21-8, Ethylamine, 2-chloro-1-methyl-, hydrochloride
(preparation of)
RN 5968-21-8 CAPLUS
CN 2-Propanamine, 1-chloro-, hydrochloride (9CI) (CA INDEX NAME)

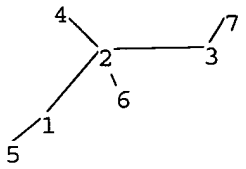


L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
AB MeCH(NMe2)CO2Et is reduced by the Bouveault-Blanc procedure to 55% of MeCH(NMe2)CH2OH (I), b. 145-8° (picrate, orange-yellow, m. 182-3°); 20 g. I in 45 cc. C6H6, added (20 min.) to 23 g. SOCl2 in 90 cc. C6H6 at 0°, allowed to warm to room temperature, and refluxed 1.5 hrs., give 59% MeCH(NMe2)CH2Cl.HCl (II), m. 103-4°. Me2NCH2CHMeOH (III) yields a picrate, orange-yellow, m. 83-4°. III (20 g.) and 23 g. SOCl2, as above, give 73% Me2NCH2CHMeCl.HCl (IV), m. 190-1°. I (20 g.) in 45 cc. C6H6, treated with 23 g. SOCl2 in 90 cc. C6H6 and the gummy residue refluxed with 150 cc. Me2CO, gives 34% IV; the II is removed by the Me2CO. 1-Piperidino-2-propanol (b762 198-201°; picrate, m. 134-5°) gives with SOCl2 2-chloro-1-(1-piperidyl)propane-HCl (V), m. 213-14°. 1-(1-Piperidyl)-3-propanol (m. 66-7°) with SOCl2 gives 1-chloro-3-(1-piperidyl)propane (VI), b10 79-80°; HCl salt, m. 213-14°. The mother liquor from V or VI did not contain the other isomer. 1-Allylpiperidine (picrate, m. 72-3°) does not add HCl. The base, Me2NCH2CHMeCl (VII), liberated from IV by dilute NH4OH at 0° or with 40% NaOH at room temperature, is stable and gives the same picrate, even after distillation (b35 36-7°). The base liberated from II at room temperature by 40% NaOH solution is Me2NCHMeCH2Cl (VIII) (Schultz, et al.,
C.A. 42, 4934i). VIII can be heated in an inert solvent and can be agitated in an inert solvent with NaOH or NaNH2 without undergoing decomposition or isomerization; on distillation in vacuo, VIII is isomerized and VII
and VIII can be separated by fractional crystallization of the picrates. The relative
proportions of the isomers formed in the alkylation of PhCH2CN with VII or V were determined by effecting as complete as possible a separation of the isomers
giving the more sparingly soluble salts. In the dimethylamino series, the N-compds. from the more sparingly soluble salts, whereas in the analogous piperidyl series, the salts of the iso compds. have the lowest solubility In
the former series at least 60% of the cyanide was formed by isolation as 6-dimethylamino-4,4-diphenyl-3-heptane-HBr and in the latter at least 45% of the isocyanide as 3-imino-5-methyl-4,4-diphenyl-6-(1-piperidyl)hexane-ZHCl. Thus, the relative proportions vary according to the nature of the basic groups of the Cl base employed in the alkylation.
ACCESSION NUMBER: 1952:5554 CAPLUS
DOCUMENT NUMBER: 46:5554
ORIGINAL REFERENCE NO.: 46:986h-i,987a-d
TITLE: Amidone. Some isomeric chlorodialkylaminopropanes and their reaction with diphenylmethyl cyanide
AUTHOR(S): Ofner, P.
CORPORATE SOURCE: Wellcome Chem. Works, Dartford, UK
SOURCE: Journal of the Chemical Society, Abstracts (1951) 1800-3
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
IT 37143-56-9, Ethylamine, 2-chloro-1-methyl-
(derivs.)
RN 37143-56-9 CAPLUS
CN 2-Propanamine, 1-chloro- (9CI) (CA INDEX NAME)



```
=>  fil reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                        141.02     302.99

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
                                                           ENTRY    SESSION
CA SUBSCRIBER PRICE                                        -20.44     -20.44

FILE 'REGISTRY' ENTERED AT 15:45:26 ON 21 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   20 MAY 2005  HIGHEST RN 850848-27-0
DICTIONARY FILE UPDATES:  20 MAY 2005  HIGHEST RN 850848-27-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\09857465.str
```



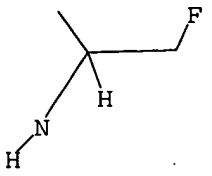

```
chain nodes :
1  2  3  4  5  6  7
chain bonds :
1-2  1-5  2-3  2-4  2-6  3-7
exact/norm bonds :
1-2
```

exact bonds :
1-5  2-3  2-4  2-6  3-7

Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS

L5      STRUCTURE UPLOADED

=> d query
L5              STR




Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 15:46:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1506 TO ITERATE

 66.4% PROCESSED    1000 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       27792 TO    32448
PROJECTED ANSWERS:           4188 TO     6112

L6           50 SEA SSS SAM L5

=> s l5 full
FULL SEARCH INITIATED 15:46:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  29640 TO ITERATE

100.0% PROCESSED   29640 ITERATIONS                      4947 ANSWERS
SEARCH TIME: 00.00.01

L7         4947 SEA SSS FUL L5

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.76     464.75

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                 0.00     -20.44

```
FILE 'CAPLUS' ENTERED AT 15:46:27 ON 21 MAY 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 21 May 2005  VOL 142 ISS 22
FILE LAST UPDATED: 20 May 2005  (20050520/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> s l7
L8         1574 L7

=> s chiral
          99396 CHIRAL
             15 CHIRALS
L9        99399 CHIRAL
                (CHIRAL OR CHIRALS)

=> s l8 and l9
L10           90 L8 AND L9

=> d l10 50-90 abs ibib hitstr
```

L10 ANSWER 50 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

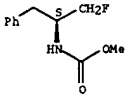
AB Chiral 2-oxazolidinones were produced in good yields by treatment of N-tert-butoxycarbonyl β-amino alcs. with Et2NSF3 (DAST) under mild reaction conditions. An intramol. nucleophilic attack mechanism is proposed to explain the formation of the heterocycles.

ACCESSION NUMBER: 1999:516282 CAPLUS
DOCUMENT NUMBER: 131:257473
TITLE: Treatment of N-Boc derivatives of β-amino alcohols with N,N-diethylaminosulfur trifluoride leads to chiral oxazolidinones. An unexpected intramolecular cyclization
AUTHOR(S): Zhao, He; Thurkauf, Andrew
CORPORATE SOURCE: Dep. Chemistry, Neurogen Corporation, Branford, CT, 06405, USA
SOURCE: Synlett (1999), (8), 1280-1282
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:257473

IT **245107-67-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of oxazolidinones by intramol. cyclocondensation of N-Boc β-amino alcs. using (ethylamino)sulfur fluoride)

RN 245107-67-9 CAPLUS
CN Carbamic acid, [(1S)-1-(fluoromethyl)-2-phenylethyl]-, methyl ester (9CI) (CA INDEX NAME)

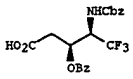
Absolute stereochemistry.



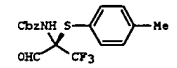
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 51 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

GI



I



II

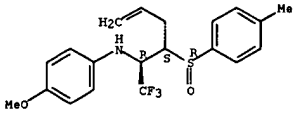
AB Two efficient approaches to both enantiomers of protected syn-γ-trifluoromethyl-γ-amino-β-hydroxybutyric acid (γ-Tfm-GABOB) (I), a new hydroxymethylene (statine) dipeptide isostere, are described. One exploits the recently disclosed 'non-oxidative' Pummerer reaction, by means of which α-lithium alkyl sulfoxides are used as chiral α-hydroxyalkyl anion equivalent in the synthesis of α-amino alcs. Trifluoropyruvaldehyde-N,S-ketal (R)-II, a novel stereochem. stable synthetic equivalent of α-amino trifluoropropanal, is used in the second approach.

ACCESSION NUMBER: 1998:805128 CAPLUS
DOCUMENT NUMBER: 130:125358
TITLE: Stereocontrolled approaches to (+)- and (-)-γ-trifluoromethyl-GABOB, a new hydroxymethylene (statine) dipeptide isostere
AUTHOR(S): Bravo, Pierfrancesco; Corradi, Eleonora; Pesenti, Cristina; Vergani, Barbara; Viani, Fiorenza; Volonterio, Alessandro; Zanda, Matteo
CORPORATE SOURCE: Centro di Studio sulle Sostanze Organiche Naturali, C.N.R, Milan, I-20131, Italy
SOURCE: Tetrahedron: Asymmetry (1998), 9(21), 3731-3735
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:125358

IT **219953-58-9P 219953-74-9P**
RL: BYP (Byproduct); PREP (Preparation)
(stereocontrolled approaches to trifluoromethyl(amino)hydroxybutyric acid stereoisomers as new hydroxymethylene (statine) dipeptide isosteres)

RN 219953-58-9 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1R,2S)-2-[(R)-(4-methylphenyl)sulfinyl]-1-(trifluoromethyl)-4-pentenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

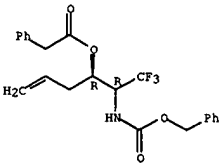


RN 219953-74-9 CAPLUS
CN Benzeneacetic acid, (1R)-1-[(1R)-2,2,2-trifluoro-1-

L10 ANSWER 51 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

[[(phenylmethoxy)carbonyl]amino]ethyl]-3-butenyl ester (9CI) (CA INDEX NAME)

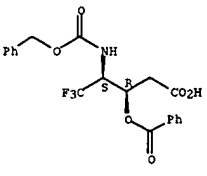
Absolute stereochemistry.



IT **219953-78-3P**
RL: PNU (Preparation, unclassified); PREP (Preparation)
(stereocontrolled approaches to trifluoromethyl(amino)hydroxybutyric acid stereoisomers as new hydroxymethylene (statine) dipeptide isosteres)

RN 219953-78-3 CAPLUS
CN D-threo-Pentonic acid, 2,4,5-trideoxy-5,5,5-trifluoro-4-[[(phenylmethoxy)carbonyl]amino]-, 3-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

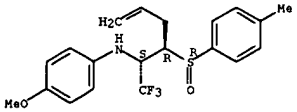


IT **219953-60-3P 219953-62-5P 219953-64-7P**
**219953-66-9P 219953-68-1P 219953-75-0P**
**219953-77-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled approaches to trifluoromethyl(amino)hydroxybutyric acid stereoisomers as new hydroxymethylene (statine) dipeptide isosteres)

RN 219953-60-3 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S,2R)-2-[(R)-(4-methylphenyl)sulfinyl]-1-(trifluoromethyl)-4-pentenyl]- (9CI) (CA INDEX NAME)

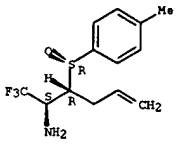
Absolute stereochemistry.

L10 ANSWER 51 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



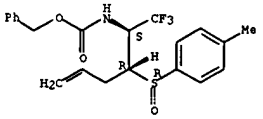
RN 219953-62-5 CAPLUS
CN 5-Hexen-2-amine, 1,1,1-trifluoro-3-[(R)-(4-methylphenyl)sulfinyl]-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



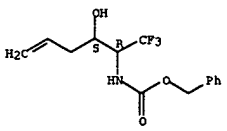
RN 219953-64-7 CAPLUS
CN Carbamic acid, [(1S,2R)-2-[(R)-(4-methylphenyl)sulfinyl]-1-(trifluoromethyl)-4-pentenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



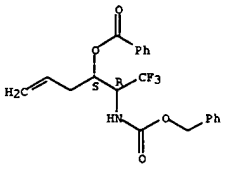
RN 219953-66-9 CAPLUS
CN Carbamic acid, [(1R,2S)-2-hydroxy-1-(trifluoromethyl)-4-pentenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



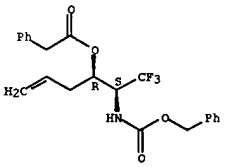
RN 219953-68-1 CAPLUS
CN Carbamic acid, [(1R,2S)-2-(benzoyloxy)-1-(trifluoromethyl)-4-pentenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 219953-75-0 CAPLUS
CN Benzeneacetic acid, (1R)-1-[(1S)-2,2,2-trifluoro-1-[[(phenylmethoxy)carbonyl]amino]ethyl]-3-butenyl ester (9CI) (CA INDEX NAME)

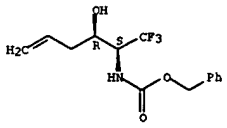
Absolute stereochemistry.



RN 219953-77-2 CAPLUS
CN Carbamic acid, [(1S,2R)-2-hydroxy-1-(trifluoromethyl)-4-pentenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

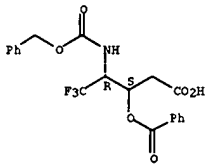
Absolute stereochemistry.





IT **219953-70-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereocontrolled approaches to trifluoromethyl(amino)hydroxybutyric acid stereoisomers as new hydroxymethylene (statine) dipeptide isosteres)
RN 219953-70-5 CAPLUS
CN L-threo-Pentonic acid, 2,4,5-trideoxy-5,5,5-trifluoro-4-{[(phenylmethoxy)carbonyl]amino}-, 3-benzoate (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

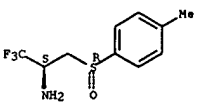


AB Asym. addition reactions between α-lithium derivs. of enantiomerically pure Me and benzyl p-tolyl sulfoxides and N-(p-methoxyphenyl)aldimines, bearing trifluoromethyl, pentafluoroethyl and α-hydrotetrafluoroethyl groups, afford α-fluoroalkyl β-sulfinylamines, synthetically versatile precursors of a series of enantiomerically pure biomedicinally important α-fluoroakylalkylamines and α-fluoroalkyl-β-hydroxyalkylamines. The addition reactions proceed under mild conditions allowing for convenient preparation of the α-fluoroalkyl β-sulfinylamines in excellent yields and good enantiomeric purity. The stereochem. outcomes of these reactions were shown to be subject to kinetic control, that is in sharp contrast to the corresponding reactions of fluorine-free imines. The absolute configurations of the addition products suggest that the fluoroalkyl group on the starting imines plays the role of an enantiodirecting, sterically larger substituent leading to transition states that are unusual for this type of reaction.

ACCESSION NUMBER: 1998:652036 CAPLUS
DOCUMENT NUMBER: 129:343304
TITLE: Chiral sulfoxide controlled asymmetric additions to C-N double bond. An efficient approach to stereochemically defined α-fluoroalkyl amino compounds
AUTHOR(S): Bravo, Pierfrancesco; Guidetti, Maurizia; Viani, Fiorenza; Zanda, Matteo; Markovsky, Andrew L.; Sorochinsky, Alexander E.; Soloshonok, Irina V.; Soloshonok, Vadim A.
CORPORATE SOURCE: C.N.R.-Centro per le Sostanze Org. Naturali, Dip. Chim. Politecnico Milano, Milano, I-20131, Italy
SOURCE: Tetrahedron (1998), 54(42), 12789-12806
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:343304

IT **169136-05-0P 182880-39-3P 189396-88-1P 189396-91-6P 189396-93-8P 189396-94-9P 189396-95-0P 215516-72-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(chiral sulfoxide controlled asym. addns. to fluoroalkyl aldimines)
RN 169138-05-0 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(R)-(4-methylphenyl)sulfinyl]-, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

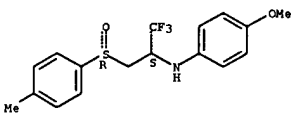


RN 182880-39-3 CAPLUS



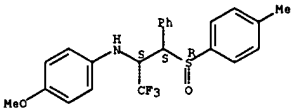
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,2-trifluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



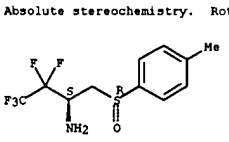
RN 189396-88-1 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(trifluoromethyl)-, (αS,βS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



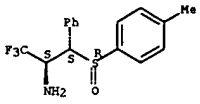
RN 189396-91-6 CAPLUS
CN 2-Butanamine, 3,3,4,4,4-pentafluoro-1-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



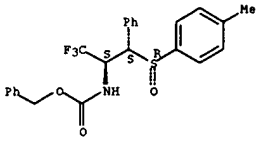
RN 189396-93-8 CAPLUS
CN Benzeneethanamine, β-[(R)-(4-methylphenyl)sulfinyl]-α-(trifluoromethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



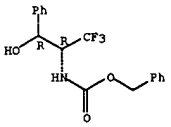
RN 189396-94-9 CAPLUS
CN Carbamic acid, [(1S)-2,2,2-trifluoro-1-[(S)-[(R)-(4-methylphenyl)sulfinyl]phenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-95-0 CAPLUS
CN Carbamic acid, [(1R)-2,2,2-trifluoro-1-[(R)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

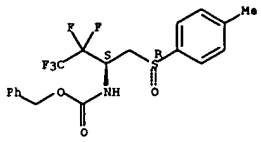
Absolute stereochemistry. Rotation (-).



RN 215516-72-6 CAPLUS
CN Carbamic acid, [(1S)-2,2,3,3,3-pentafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).





IT 177469-12-4P 189350-65-0P 189396-86-9P
189396-87-0P 189396-89-2P 189396-90-5P
189396-92-7P 189396-96-1P 215516-67-9P
215516-69-1P 215516-70-4P 215516-74-8P
215516-76-0P 215516-77-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(chiral sulfoxide controlled asym. addns. to fluoroalkyl aldimines)

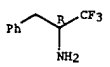
RN 177469-12-4 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 189350-65-0 CAPLUS
CN Benzeneethanamine, α-(trifluoromethyl)-, hydrochloride, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

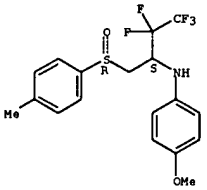


● HCl

RN 189396-86-9 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,3,3,3-pentafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

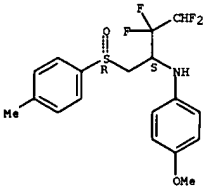
Absolute stereochemistry. Rotation (+).





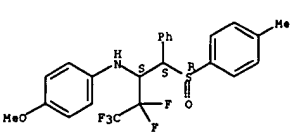
RN 189396-87-0 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,3,3-tetrafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-89-2 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(pentafluoroethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

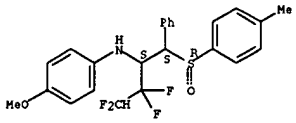


RN 189396-90-5 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(1,1,2,2-tetrafluoroethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

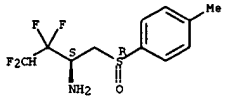






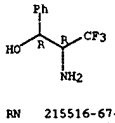
RN 189396-92-7 CAPLUS
CN 2-Butanamine, 3,3,4,4-tetrafluoro-1-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



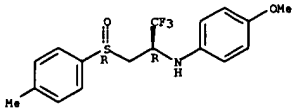
RN 189396-96-1 CAPLUS
CN Benzenemethanol, α-[(1R)-1-amino-2,2,2-trifluoroethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



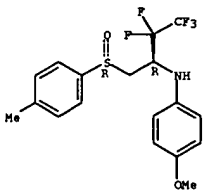
RN 215516-67-9 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1R)-2,2,2-trifluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



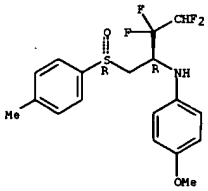
RN 215516-69-1 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1R)-2,2,3,3,3-pentafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



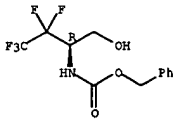
RN 215516-70-4 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1R)-2,2,3,3-tetrafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 215516-74-8 CAPLUS
CN Carbamic acid, [(1R)-2,2,3,3,3-pentafluoro-1-(hydroxymethyl)propyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

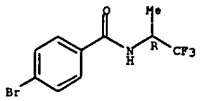
Absolute stereochemistry. Rotation (-).



RN 215516-76-0 CAPLUS
CN Benzamide, 4-bromo-N-[(1R)-2,2,2-trifluoro-1-methylethyl]- (9CI) (CA INDEX NAME)

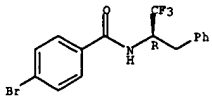


Absolute stereochemistry. Rotation (+).



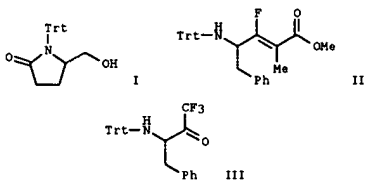
RN 215516-77-1 CAPLUS
CN Benzamide, 4-bromo-N-[(1R)-2,2,2-trifluoro-1-(phenylmethyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 53 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB Cyanuric fluoride-mediated fluorination of chiral N-tritylamino acids leads to the corresponding acyl fluorides which are powerful acylating agents for peptide synthesis. The acyl fluorides react with NaBH4, the stabilized phosphorane Ph3P:C(Me)CO2Me, and Ruppert's reagent providing access to enantiomerically pure trityl amino alcs., e.g. I (Trt = Ph3C), alkenes, e.g. II, and trifluoromethyl ketones, e.g. III, resp.

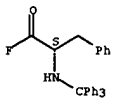
ACCESSION NUMBER: 1998:608120 CAPLUS
DOCUMENT NUMBER: 129:290399
TITLE: Preparation and properties of enantiomerically pure Nα-tritylamino acid fluorides
AUTHOR(S): Karygiannis, Georgios; Athanassopoulos, Costas; Mamos, Petros; Karamanos, Nikolaos; Papaioannou, Dionissios; Francis, George W.
CORPORATE SOURCE: Department of Chemistry, University of Patras, Patras, 265 00, Greece
SOURCE: Acta Chemica Scandinavica (1998), 52(9), 1144-1150
CODEN: ACHSE7; ISSN: 0904-213X
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:290399

IT **214344-15-7P 214344-16-8P 214344-17-9P 214344-23-7DP**, resin bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of enantiomerically pure trityl amino acid fluorides)

RN 214344-15-7 CAPLUS
CN Benzenepropanoyl fluoride, α-[(triphenylmethyl)amino]-, (αS)- (9CI) (CA INDEX NAME)

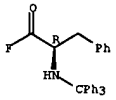
Absolute stereochemistry. Rotation (+).





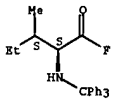
RN 214344-16-8 CAPLUS
CN Benzenepropanoyl fluoride, α-[(triphenylmethyl)amino]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



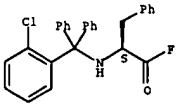
RN 214344-17-9 CAPLUS
CN Pentanoyl fluoride, 3-methyl-2-[(triphenylmethyl)amino]-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 214344-23-7 CAPLUS
CN Benzenepropanoyl fluoride, α-[[(2-chlorophenyl)diphenylmethyl]amino]-, (αS)- (9CI) (CA INDEX NAME)

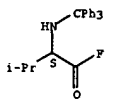
Absolute stereochemistry.



IT **214344-18-0P 214344-19-1P 214344-31-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of enantiomerically pure trityl amino acid fluorides)

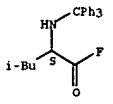
L10 ANSWER 53 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 214344-18-0 CAPLUS
CN Butanoyl fluoride, 3-methyl-2-[(triphenylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



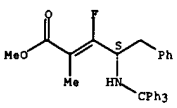
RN 214344-19-1 CAPLUS
CN Pentanoyl fluoride, 4-methyl-2-[(triphenylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 214344-31-7 CAPLUS
CN 2-Pentenoic acid, 3-fluoro-2-methyl-5-phenyl-4-[(triphenylmethyl)amino]-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

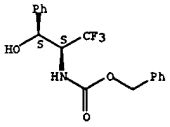
Absolute stereochemistry.
Double bond geometry unknown.



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 54 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB A new, efficient, and stereoselective two-step approach to stereochem. defined chiral nonracemic γ-tri- and γ-difluoro β-amino alcs. (70% to >95% ee) is described, using tri- and difluoropyruvaldehyde N,S-ketals (R)-4-MeC6H4SC(CHO)(R)NHCO2CH2Ph [I, R = CF3, CHF2] as starting materials. Addition of Grignard reagents to I occurs with moderate to excellent anti stereocontrol, depending on the nature of the organomagnesium halides, providing the β-p-tolylthio β-benzyloxycarbonylamino secondary carbinols. The stereochem. outcome of these reactions can be rationalized by means of a chelated Cram's cyclic model, where the NCbz group is the chelating ligand and the p-tolylthio residue acts as the stereocontrolling large group. Reductive displacement of the 2-p-tolylthio substituent efficiently takes places by means of the NaBH4/pyridine system, probably via intermediate transient imines, providing sulfur-free γ-tri- and γ-difluorinated β-amino alcs. with high levels of anti-stereoselectivity. A considerable shift toward syn-stereoselectivity was obtained performing the reaction on the corresponding phenylacetates. Cleavage and reduction of the NHCbz moiety of the fluorinated β-amino alcs. provided tri- and difluoro analogs of, resp., norephedrine and ephedrine.
ACCESSION NUMBER: 1998:603684 CAPLUS
DOCUMENT NUMBER: 129:316007
TITLE: (R)-Trifluoro- and Difluoropyruvaldehyde N,S-Ketals: Chiral Synthetic Equivalents of β-Trifluoro and β-Difluoro α-Amino Aldehydes
AUTHOR(S): Volonterio, Alessandro; Vergani, Barbara; Crucianelli, Marcello; Zanda, Matteo; Bravo, Pierfrancesco
CORPORATE SOURCE: Dipartimento di Chimica del Politecnico, Milan, I-20131, Italy
SOURCE: Journal of Organic Chemistry (1998), 63(21), 7236-7243 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:316007
IT **188566-32-7P 214852-75-2P 214852-77-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of fluoro amino alcs. from fluoropyruvaldehyde N,S-ketals)
RN 188566-32-7 CAPLUS
CN Carbamic acid, [(1S)-2,2,2-trifluoro-1-[(S)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

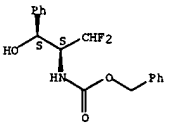
Absolute stereochemistry. Rotation (+).



RN 214852-75-2 CAPLUS

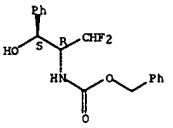
L10 ANSWER 54 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Carbamic acid, [(1S)-2,2-difluoro-1-[(S)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



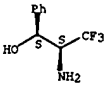
RN 214852-77-4 CAPLUS
CN Carbamic acid, [(1R)-2,2-difluoro-1-[(S)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **188566-33-8P 188566-34-9P 214852-69-4P**
**214852-70-7P 214852-71-8P 214852-72-9P**
**214852-73-0P 214852-74-1P 214852-79-6P**
**214852-80-9P 214852-82-1P 214852-84-3P**
**214852-85-4P 214852-86-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of fluoro amino alcs. from fluoropyruvaldehyde N,S-ketals)
RN 188566-33-8 CAPLUS
CN Benzenemethanol, α-[(1S)-1-amino-2,2,2-trifluoroethyl]-, (αS)- (9CI) (CA INDEX NAME)

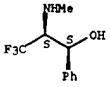
Absolute stereochemistry. Rotation (+).



RN 188566-34-9 CAPLUS
CN Benzenemethanol, α-[(1S)-2,2,2-trifluoro-1-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

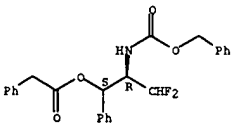
L10 ANSWER 54 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).



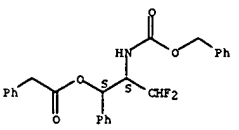
RN 214852-69-4 CAPLUS
CN Benzeneacetic acid, (1S,2R)-3,3-difluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



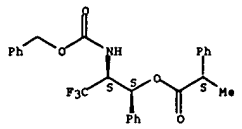
RN 214852-70-7 CAPLUS
CN Benzeneacetic acid, (1S,2S)-3,3-difluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



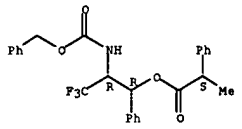
RN 214852-71-8 CAPLUS
CN Benzeneacetic acid, α-methyl-, (1S,2S)-3,3,3-trifluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



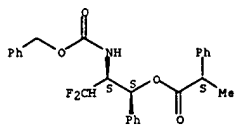
RN 214852-72-9 CAPLUS
CN Benzeneacetic acid, α-methyl-, (1R,2R)-3,3,3-trifluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214852-73-0 CAPLUS
CN Benzeneacetic acid, α-methyl-, (1S,2S)-3,3-difluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



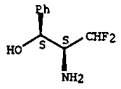
RN 214852-74-1 CAPLUS
CN Benzeneacetic acid, α-methyl-, (1R,2R)-3,3-difluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



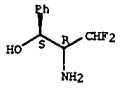
RN 214852-84-3 CAPLUS
CN Benzenemethanol, α-[(1S)-1-amino-2,2-difluoroethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



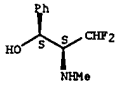
RN 214852-85-4 CAPLUS
CN Benzenemethanol, α-[(1R)-1-amino-2,2-difluoroethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



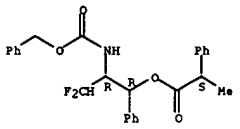
RN 214852-86-5 CAPLUS
CN Benzenemethanol, α-[(1S)-2,2-difluoro-1-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



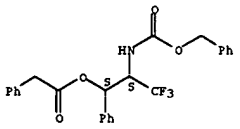
REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT





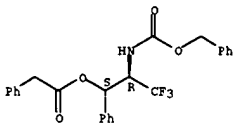
RN 214852-79-6 CAPLUS
CN Benzeneacetic acid, (1S,2S)-3,3,3-trifluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



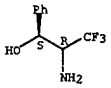
RN 214852-80-9 CAPLUS
CN Benzeneacetic acid, (1S,2R)-3,3,3-trifluoro-1-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 214852-82-1 CAPLUS
CN Benzenemethanol, α-[(1R)-1-amino-2,2,2-trifluoroethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





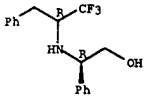
AB Chiral 1,3-oxazolidinones, obtained from RCOCF3 [R = Ph, CH2Ph] and (R)-phenylglycinol, underwent asym. reduction with LiAlH4 to give F3CCHRNHCHPhCH2OH with retention of configuration.

ACCESSION NUMBER: 1998:111686 CAPLUS
DOCUMENT NUMBER: 128:180188
TITLE: Stereospecific reduction with retention of chiral fluoral-derived 1,3-oxazolidines with LiAlH4: asymmetric synthesis of 1-substituted 2,2,2-trifluoroethylamines
AUTHOR(S): Ishii, Akihiro; Miyamoto, Fumie; Higashiyama, Kimio; Mikami, Koichi
CORPORATE SOURCE: Department of Chemical Technology, Tokyo Institute of Technology, Tokyo, 152, Japan
SOURCE: Chemistry Letters (1998), (2), 119-120
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:180188

IT **203176-66-3P 203258-91-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and stereoselective reduction of chiral oxazolidines derived from trifluoromethyl ketones)

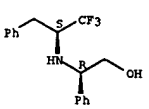
RN 203176-66-3 CAPLUS
CN Benzeneethanol, β-[[(1R)-2,2,2-trifluoro-1-(phenylmethyl)ethyl]amino]-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 203258-91-7 CAPLUS
CN Benzeneethanol, β-[[(1S)-2,2,2-trifluoro-1-(phenylmethyl)ethyl]amino]-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 56 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

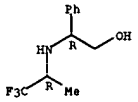
AB The synthesis of 1-substituted 2,2,2-trifluoroethylamines starting from chiral fluoral hemiacetals derived from fluoral and (R)-phenylglycinol is decribed. The asym. addition reactions of Grignard reagents to the resultant imine are used in the key reaction step.

ACCESSION NUMBER: 1998:47953 CAPLUS
DOCUMENT NUMBER: 128:180181
TITLE: Asymmetric addition reactions of Grignard reagents to chiral fluoral hemiacetal. Asymmetric synthesis of 1-substituted 2,2,2-trifluoroethylamines
AUTHOR(S): Ishii, Akihiro; Higashiyama, Kimio; Mikami, Koichi
CORPORATE SOURCE: Dep. Chemical Technology, Tokyo Inst. Technology, Tokyo, 152, Japan
SOURCE: Synlett (1997), (12), 1381-1382
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:180181

IT **203176-64-1P 203176-66-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (fluoroethyl)amines by asym. Grignard reaction of fluoral hemiacetal)

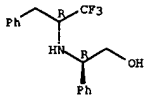
RN 203176-64-1 CAPLUS
CN Benzeneethanol, β-[[(2,2,2-trifluoro-1-methylethyl)amino]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



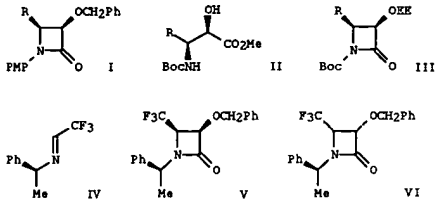
RN 203176-66-3 CAPLUS
CN Benzeneethanol, β-[[(1R)-2,2,2-trifluoro-1-(phenylmethyl)ethyl]amino]-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 57 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

GI



AB Cycloaddn. of the (fluoroalkyl)imines RCH:N-PMP (R = CF3, CF2H, CF2Cl; PMP = 4-MeOC6H4) with the ketene formed in situ from (benzyloxy)acetyl chloride and triethylamine provided stereoselectively cis-(fluoroalkyl)azetidinones I in moderate yields. The corresponding N-Boc-isoserinates II (Boc = Me3CO2C) and protected synthons III (EE = 2-ethoxyethyl) have been prepared from these azetidinones I. Cycloaddn. of the chiral imine IV with the same ketene led to the diastereoisomeric azetidinones V and VI with a poor diastereoisomeric excess (10-20%). However, the two diastereoisomers could be easily separated by crystallization and provided enantiomerically pure N-Boc-isoserinates (R,R)- and (S,S)-II (R = CF3) after ring opening and debenzylation.

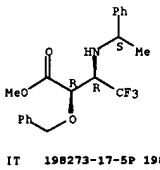
ACCESSION NUMBER: 1997:786534 CAPLUS
DOCUMENT NUMBER: 127:359060
TITLE: Diastereoselective Synthesis of the Nonracemic Methyl syn-(3-Fluoroalkyl)isoserinates
AUTHOR(S): Abouabdellah, Ahmed; Begue, Jean-Pierre; Bonnet-Delpon, Daniele; Nga, Truong Thi Thanh
CORPORATE SOURCE: Centre d'Etudes Pharmaceutiques, CNRS, Chatenay-Malabry, 92296, Fr.
SOURCE: Journal of Organic Chemistry (1997), 62(25), 8826-8833
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:359060

IT **198273-25-5P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereoselective synthesis of nonracemic syn-(fluoroalkyl)isoserine Me esters)

RN 198273-25-5 CAPLUS
CN Butanoic acid, 4,4,4-trifluoro-3-[[(1S)-1-phenylethyl]amino]-2-(phenylmethoxy)-, methyl ester, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

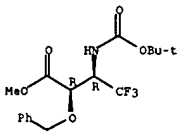
L10 ANSWER 57 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **198273-17-5P 198273-18-6P 198273-26-6P**
**198273-32-4P 198273-33-5P 198273-41-5P**
**198273-42-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(diastereoselective synthesis of nonracemic syn-(fluoroalkyl)isoserine Me esters)

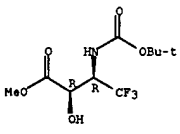
RN 198273-17-5 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-(phenylmethoxy)-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 198273-18-6 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

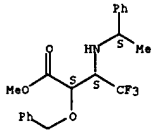
Relative stereochemistry.



RN 198273-26-6 CAPLUS
CN Butanoic acid, 4,4,4-trifluoro-3-[[(1S)-1-phenylethyl]amino]-2-(phenylmethoxy)-, methyl ester, (2S,3S)- (9CI) (CA INDEX NAME)

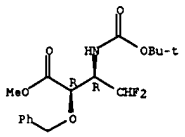
Absolute stereochemistry. Rotation (-).

L10 ANSWER 57 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



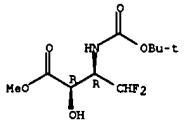
RN 198273-32-4 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-difluoro-2-(phenylmethoxy)-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 198273-33-5 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-difluoro-2-hydroxy-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

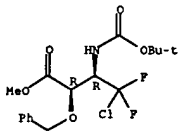
Relative stereochemistry.



RN 198273-41-5 CAPLUS
CN Butanoic acid, 4-chloro-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-difluoro-2-(phenylmethoxy)-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

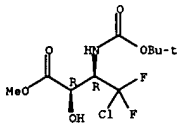
Relative stereochemistry.

L10 ANSWER 57 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



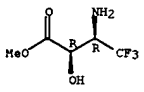
RN 198273-42-6 CAPLUS
CN Butanoic acid, 4-chloro-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4-difluoro-2-hydroxy-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **177838-12-9P 198273-27-7P 198273-28-8P**
**198273-36-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereoselective synthesis of nonracemic syn-(fluoroalkyl)isoserine Me esters)
RN 177838-12-9 CAPLUS
CN Butanoic acid, 3-amino-4,4,4-trifluoro-2-hydroxy-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

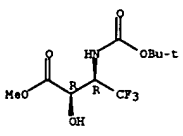
Relative stereochemistry.



RN 198273-27-7 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, methyl ester, (2R,3R)- (9CI) (CA INDEX NAME)

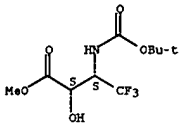
Absolute stereochemistry. Rotation (-).

L10 ANSWER 57 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



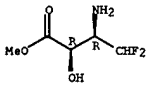
RN 198273-28-8 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, methyl ester, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



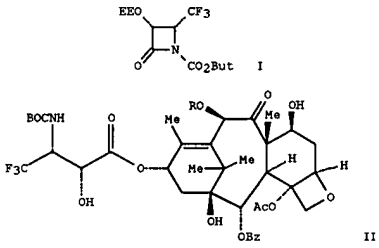
RN 198273-36-8 CAPLUS
CN Butanoic acid, 3-amino-4,4-difluoro-2-hydroxy-, methyl ester, (2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

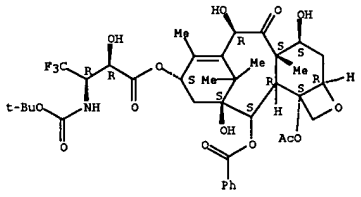
L10 ANSWER 58 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB The coupling of racemic 4-CF3-β-lactam (I) with various C-10 modified baccatins has resulted in CF3-taxoids (II) (R = H, Ac, Me2NCO, cyclopropanecarbonyl, MeO2C, 4-morpholinecarbonyl, EtCO, BuCO, Me3CCH2CO) with diastereoselectivities ranging from 9:1 to one single isomer. The observed high diastereoselectivity is ascribed to the highly efficient enantiomer-differentiation by the enantiopure lithium alkoxide of a baccatin III in the coupling reaction with a racemic 1-tBoc-β-lactam. These novel CF3-taxoids have also been shown to exhibit significant increases in activity against various cancer cell lines compared to either paclitaxel or docetaxel. In addition, the first asym. synthesis of a CF3-β-lactam via chiral ester enolate-imine cyclocondensation was performed with 50% enantioselectivity.
ACCESSION NUMBER: 1997:652772 CAPLUS
DOCUMENT NUMBER: 127:293438
TITLE: Synthesis of novel 3'-trifluoromethyl taxoids through effective kinetic resolution of racemic 4-CF3-β-lactams with baccatins
AUTHOR(S): Ojima, Iwao; Slater, John C.
CORPORATE SOURCE: Department of Chemistry, State University of New York at Stony Brook, Stony Brook, NY, 11794-3400, USA
SOURCE: Chirality (1997), 9(5/6), 487-494
CODEN: CHRLEP; ISSN: 0899-0042
PUBLISHER: Wiley-Liss
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:293438
IT **186819-41-0P 186819-42-1P 186819-43-2P**
**186819-44-3P 186819-45-4P 186819-46-5P**
**186819-47-6P 186819-48-7P 186819-49-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of 3'-trifluoromethyl taxoids through kinetic resolution of racemic 4-CF3-β-lactams with baccatins)

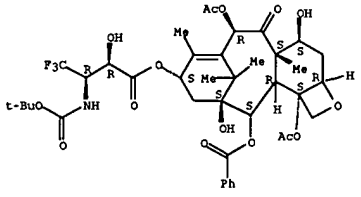
L10 ANSWER 58 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 186819-41-0 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



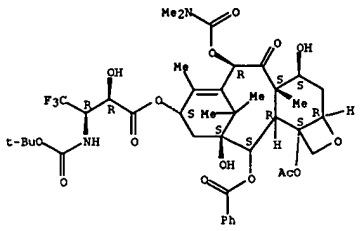
RN 186819-42-1 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



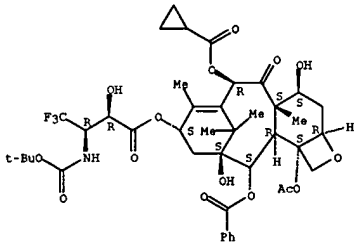
RN 186819-43-2 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-6-[[(dimethylamino)carbonyl]oxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 186819-44-3 CAPLUS
CN Cyclopropanecarboxylic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[(2R,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-1-oxobutoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

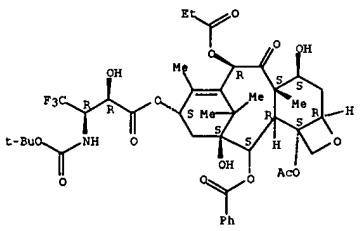
Absolute stereochemistry. Rotation (-).



RN 186819-45-4 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-6-[(methoxycarbonyl)oxy]-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

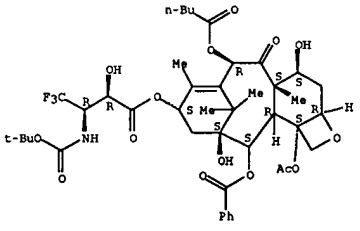
Absolute stereochemistry. Rotation (-).





RN 186819-48-7 CAPLUS
CN Pentanoic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[(2R,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-1-oxobutoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

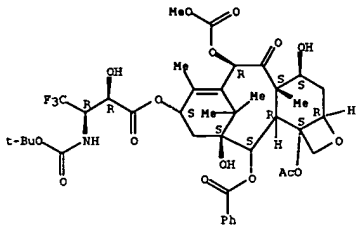
Absolute stereochemistry. Rotation (-).



RN 186819-49-8 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-6-(3,3-dimethyl-1-oxobutoxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

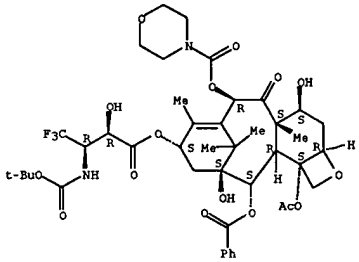
Absolute stereochemistry. Rotation (-).





RN 186819-46-5 CAPLUS
CN 4-Morpholinecarboxylic acid, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-9-[(2R,3R)-3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-1-oxobutoxy]-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-6-yl ester (9CI) (CA INDEX NAME)

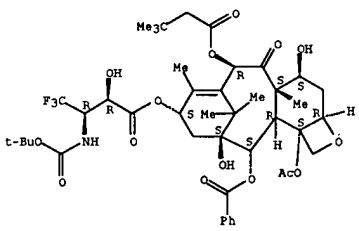
Absolute stereochemistry. Rotation (-).



RN 186819-47-6 CAPLUS
CN Butanoic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-4,4,4-trifluoro-2-hydroxy-, (2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-tetramethyl-5-oxo-6-(1-oxopropoxy)-7,11-methano-1H-cyclodeca[3,4]benz[1,2-b]oxet-9-yl ester, (2R,3R)- (9CI) (CA INDEX NAME)

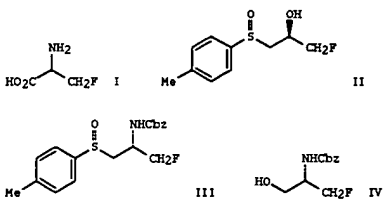
Absolute stereochemistry. Rotation (-).





REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

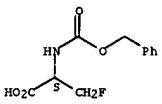
L10 ANSWER 59 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



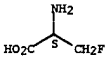
AB The wide spectrum antibacterial 3-fluoro-D-alanine (I) has been stereoselectively synthesized via chiral sulfoxide chemical. Key steps are the azidation of the α-fluoro α'-sulfinyl alc. II under Mitsunobu conditions and the one-pot transformation of protected α-sulfinyl amine III (Cbz = CO2CH2Ph) into protected amino alc. IV through a non-oxidative Pummerer reaction.

ACCESSION NUMBER: 1997:634119 CAPLUS
DOCUMENT NUMBER: 127:293573
TITLE: Stereoselective synthesis of the antibacterial 3-fluoro-D-alanine
AUTHOR(S): Bravo, Pierfrancesco; Cavicchio, Giancarlo; Crucianelli, Marcello; Poggiali, Andrea; Zanda, Matteo
CORPORATE SOURCE: Dep. Chimica Politecnico Milana, CNR Centro Studio Sostanze Organiche Naturali, Milan, I-20131, Italy
SOURCE: Tetrahedron: Asymmetry (1997), 8(16), 2811-2815
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:293573
IT **36369-37-6P 197085-99-7P 197086-00-3P 197086-01-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective synthesis of the antibacterial fluoroalanine)
RN 36369-37-6 CAPLUS
CN D-Alanine, 3-fluoro-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



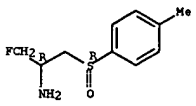
L10 ANSWER 59 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

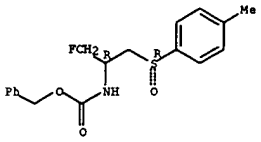
L10 ANSWER 59 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 197085-99-7 CAPLUS
CN 2-Propanamine, 1-fluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



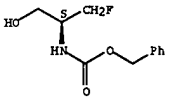
RN 197086-00-3 CAPLUS
CN Carbamic acid, [1-(fluoromethyl)-2-[(4-methylphenyl)sulfinyl]ethyl]-, phenylmethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 197086-01-4 CAPLUS
CN Carbamic acid, [2-fluoro-1-(hydroxymethyl)ethyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

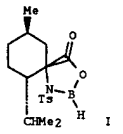
Absolute stereochemistry. Rotation (+).



IT **35455-20-0P**, 3-Fluoro-D-alanine
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective synthesis of the antibacterial fluoroalanine)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

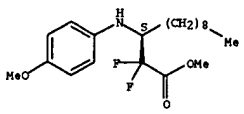
L10 ANSWER 60 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



AB Aldol reaction of aldehydes with F2C:C(OEt)OSiMe3 in the presence of a substoichiometric amount of a chiral Lewis acid provides HOCHRCF2CO2Et [R = Ph, (E)-PhCH:CH, PhCH2CH2, PhCH2OCH2, cyclohexyl, Pr, nonyl, Me2CHCH2, Et2CH] with high enantioselectivities (up to 98% ee). Reaction temperature has a great influence on the enantiofacial selection of the aldehydes; the reactions of benzyloxyacetaldehyde catalyzed by Lewis acid I at -78 and -30°C gave (+)- and (-)-PhCH2OCH2CH(OH)CF2CO2Et in optical yields of 98% and 85%, resp.

ACCESSION NUMBER: 1997:497502 CAPLUS
DOCUMENT NUMBER: 127:205149
TITLE: Asymmetric aldol addition of aldehydes to a difluoroketene silyl acetal catalyzed by chiral Lewis acids
AUTHOR(S): Iseki, Katsuhiko; Kuroki, Yoshichika; Asada, Daisuke; Takahashi, Mie; Kishimoto, Satoshi; Kobayashi, Yoshiro
CORPORATE SOURCE: MEC Laboratory, Daikin Industries, Ltd., Tsukuba, 305, Japan
SOURCE: Tetrahedron (1997), 53(30), 10271-10280
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **194421-17-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. aldol addition of aldehydes to a difluoroketene silyl acetal catalyzed by chiral Lewis acids)
RN 194421-17-5 CAPLUS
CN Dodecanoic acid, 2,2-difluoro-3-[(4-methoxyphenyl)amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS

L10 ANSWER 60 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 61 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

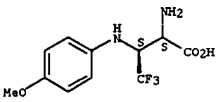
AB The LiCl/base-assisted asym. aldol-type addition reaction between the N-(p-methoxyphenyl)imine of trifluoroacetaldehyde and the chiral non-racemic Ni(II) complex of the Schiff base of glycine with (S)-o-[N-(n-benzylprolyl)amino]benzophenone was found to proceed with excellent chemical and stereochem. outcomes, allowing for an efficient access to hitherto unknown stereochem. defined β-perfluoroalkyl-α,β-diamino carboxylic acids. A mechanistic rationale for the observed stereochem. preferences is proposed.

ACCESSION NUMBER: 1997:433086 CAPLUS
DOCUMENT NUMBER: 127:149358
TITLE: Highly diastereoselective aza-aldol reactions of a chiral Ni(II) complex of glycine with imines. An efficient asymmetric approach to 3-perfluoroalkyl-2,3-diamino acids
AUTHOR(S): Soloshonok, Vadim A.; Avilov, Dimitry V.; Kukhar, Valery P.; Van Meervelt, Luc; Mischenko, Nikolai
CORPORATE SOURCE: Natl. Ind. Res. Inst. Nagoya, Nagoya City, 462, Japan
SOURCE: Tetrahedron Letters (1997), 38(26), 4671-4674
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:149358

IT **193343-11-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. approach to perfluoroalkyl diamino acids via diastereoselective aza-aldol reaction of chiral Ni(II) complex of glycine with imines)

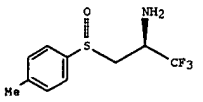
RN 193343-11-2 CAPLUS
CN Butanoic acid, 2-amino-4,4,4-trifluoro-3-[(4-methoxyphenyl)amino]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 62 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

AB Condensations between chiral α-lithiated alkyl p-tolyl sulfoxides and N-PMP fluoroalkyl aldimines (PMP = p-MeOC6H4) have been found to proceed with high simple and facial diastereoselection, providing an efficient approach to enantiomerically pure fluoro amino compds. of synthetic and biomedicinal importance. E.g., lithiation of (R)-4-MeC6H4S(O)Me, followed by addition of CF3CH:NC6H4OMe, and subsequent treatment with CAN gave sulfinyl amine I.

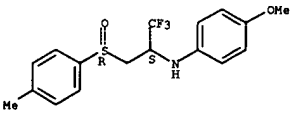
ACCESSION NUMBER: 1997:315002 CAPLUS
DOCUMENT NUMBER: 126:317207
TITLE: Stereoselective Additions of α-Lithiated Alkyl-p-tolylsulfoxides to N-PMP(fluoroalkyl)aldimines. An Efficient Approach to Enantiomerically Pure Fluoro Amino Compounds
AUTHOR(S): Bravo, Pierfrancesco; Farina, Alessandra; Kukhar, Valery P.; Markovsky, Andrey L.; Meille, Stefano V.; Soloshonok, Vadim A.; Sorochinsky, Alexander E.; Viani, Fiorenza; Zanda, Matteo; Zappala, Carmela
CORPORATE SOURCE: Dipartimento di Chimica del Politecnico, C.N.R.-Centro di Studio per le Sostanze Organiche Naturali, Milan, I-20131, Italy
SOURCE: Journal of Organic Chemistry (1997), 62(11), 3424-3425
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:317207

IT **182880-39-3P 189396-86-9P 189396-87-0P**
**189396-88-1P 189396-92-7P 189396-93-8P**
**189396-94-9P 189396-95-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective addns. of lithiated alkyl tolyl sulfoxides to fluoroalkyl aldimines)

RN 182880-39-3 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,2-trifluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

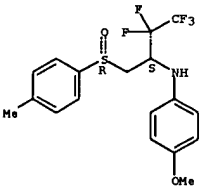
Absolute stereochemistry. Rotation (+).

L10 ANSWER 62 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



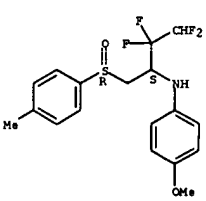
RN 189396-86-9 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,3,3,3-pentafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-87-0 CAPLUS
CN Benzenamine, 4-methoxy-N-[(1S)-2,2,3,3-tetrafluoro-1-[[(R)-(4-methylphenyl)sulfinyl]methyl]propyl]- (9CI) (CA INDEX NAME)

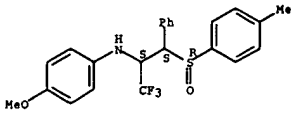
Absolute stereochemistry. Rotation (+).



RN 189396-88-1 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(trifluoromethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

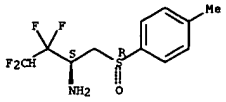
Absolute stereochemistry. Rotation (+).

L10 ANSWER 62 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



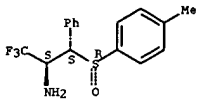
RN 189396-92-7 CAPLUS
CN 2-Butanamine, 3,3,4,4-tetrafluoro-1-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



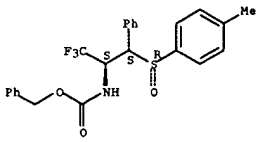
RN 189396-93-8 CAPLUS
CN Benzeneethanamine, β-[(R)-(4-methylphenyl)sulfinyl]-α-(trifluoromethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



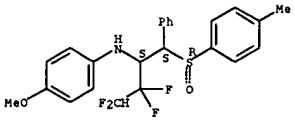
RN 189396-94-9 CAPLUS
CN Carbamic acid, [(1S)-2,2,2-trifluoro-1-[(S)-[(R)-(4-methylphenyl)sulfinyl]phenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



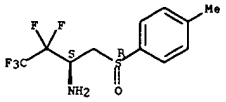
L10 ANSWER 62 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).



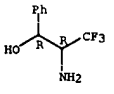
RN 189396-91-6 CAPLUS
CN 2-Butanamine, 3,3,4,4,4-pentafluoro-1-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-96-1 CAPLUS
CN Benzenemethanol, α-[(1R)-1-amino-2,2,2-trifluoroethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

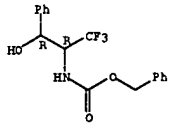


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 62 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

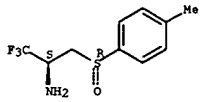
RN 189396-95-0 CAPLUS
CN Carbamic acid, [(1R)-2,2,2-trifluoro-1-[(R)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



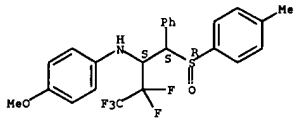
IT **169138-05-0P 189396-89-2P 189396-90-5P**
**189396-91-6P 189396-96-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective addns. of lithiated alkyl tolyl sulfoxides to fluoroalkyl aldimines)
RN 169138-05-0 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-89-2 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(pentafluoroethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 189396-90-5 CAPLUS
CN Benzeneethanamine, N-(4-methoxyphenyl)-β-[(R)-(4-methylphenyl)sulfinyl]-α-(1,1,2,2-tetrafluoroethyl)-, (αS,βS)- (9CI) (CA INDEX NAME)

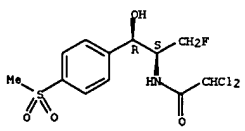
L10 ANSWER 63 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

AB Boron enolates derived from α-heterosubstituted thioacetates and bearing menthone-derived chiral ligands react with aldehydes to give anti aldols with excellent diastereo- and enantiocontrol. Boron enolates derived from tert-Bu α-halothioacetate and bearing menthone-derived chiral ligands react with imines with excellent diastereo- and enantiocontrol to give syn α-halo-β-aminothioesters, which can be converted to the corresponding aziridines by simple ring closure during LAH reduction. A key precursor of antibiotics (+)-thiamphenicol and (-)-florfenicol was synthesized.

ACCESSION NUMBER: 1997:271411 CAPLUS
DOCUMENT NUMBER: 127:17234
TITLE: Highly enantio- and diastereoselective boron aldol reactions of α-heterosubstituted thioacetates with aldehydes and silyl imines
AUTHOR(S): Gennari, Cesare; Vulpetti, Anna; Pain, Gilles
CORPORATE SOURCE: Dip. Chimica Organica, Industriale, Univ. Milano, Centro CNR Sost. Org. Nat., Milan, 20133, Italy
SOURCE: Tetrahedron (1997), 53(16), 5909-5924
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:17234

IT **73231-34-2P**, (-)-Florfenicol
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of aldols by enantio- and diastereoselective boron aldol reactions of α-heterosubstituted thioacetates with aldehydes)
RN 73231-34-2 CAPLUS
CN Acetamide, 2,2-dichloro-N-[(1S,2R)-1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 105 THERE ARE 105 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 64 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

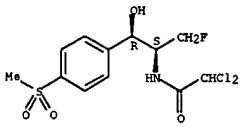
AB Improved synthesis of florfenicol and thiamphenicol, broad spectrum antibiotics, was developed and scaled up successfully in the plant. The 1'-dichloromethyloxazoline was established as a key intermediate in the new synthesis. Two methods are described here for the synthesis of florfenicol, i.e., the direct condensation of aminodiol with $CHCl_2CN$ and an enantioselective synthesis. A cost-effective one-pot inversion of the benzylic chiral center in 3'-(S,R)-oxazoline to its (R,R)-isomer is reported. A novel one-step $ZnCl_2$-promoted opening of 2,3-epoxy-1-ol was discovered to form 3'-(S,R)-oxazoline. The desired two R chiral centers in were obtained via two consecutive SN2 displacement reactions. The starting two S chiral centers were obtained from the Sharpless epoxidn.

ACCESSION NUMBER: 1997:253933 CAPLUS
DOCUMENT NUMBER: 126:252646
TITLE: An Improved Industrial Synthesis of Florfenicol plus an Enantioselective Total Synthesis of Thiamphenicol and Florfenicol
AUTHOR(S): Wu, Guangzhong; Schumacher, Doris P.; Tormos, Wanda; Clark, Jon E.; Murphy, Bruce L.
CORPORATE SOURCE: Chemical Process Research and Development, Schering-Plough Research Institute, Kenilworth, NJ, 07033, USA
SOURCE: Journal of Organic Chemistry (1997), 62(9), 2996-2998
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **73231-34-2P**, Florfenicol
RL: IMF (Industrial manufacture); PREP (Preparation)
(industrial-scale resolution-based synthesis of florfenicol and enantioselective total synthesis of thiamphenicol and florfenicol)

RN 73231-34-2 CAPLUS
CN Acetamide, 2,2-dichloro-N-[(1S,2R)-1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 65 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

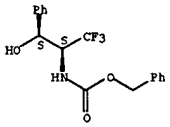
AB Chiral aldehyde, (+)-(R)-F3CC(NHCO2CH2Ph)(SC6H4-Me-4)CHO, a new trifluoro 3-carbon building block, was reacted with several Grignard reagents, RMgX, to stereoselectively afford the corresponding anti-carbamates, F3CCR(NHCO2CH2Ph)(SC6H4-Me-4)CSH(OH)R (I; R = Me, Et, vinyl, Ph). The N,S-ketal stereo center, whose absolute stereochem. was determined by x-ray anal. of the (+)-(S)-α-phenylpropionate ester of I (R = Me), was able to provide excellent stereocontrol. I (R = Ph) was further transformed to (1S,2S)-3,3,3-trifluoroephedrine and (1S,1S)-N-nor-3,3,3-trifluoroephedrine.

ACCESSION NUMBER: 1997:188006 CAPLUS
DOCUMENT NUMBER: 126:238522
TITLE: N-Cbz-trifluoropyruvaldehyde N,s-ketal: absolute stereochemistry and addition of Grignard reagents. Highly stereoselective entry to trifluoro analogs of Ephedra alkaloids
AUTHOR(S): Volonterio, Alessandro; Bravo, Pierfrancesco; Stefano, Silvia Capelli; Meille, Stefano V.; Zanda, Matteo
CORPORATE SOURCE: Dipartimento Chimica Politecnico, Centro Studio Sostanze Organiche Naturali, Milan, I-20131, Italy
SOURCE: Tetrahedron Letters (1997), 38(10), 1847-1850
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:238522

IT **188566-32-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of trifluoroephedrine analogs via stereoselective Grignard reactions with chiral trifluoropropanal)

RN 188566-32-7 CAPLUS
CN Carbamic acid, [(1S)-2,2,2-trifluoro-1-[(S)-hydroxyphenylmethyl]ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

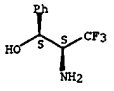


IT **188566-33-8P 188566-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of trifluoroephedrine analogs via stereoselective Grignard reactions with chiral trifluoropropanal)

RN 188566-33-8 CAPLUS
CN Benzenemethanol, α-[(1S)-1-amino-2,2,2-trifluoroethyl]-, (αS)- (9CI) (CA INDEX NAME)

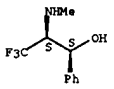
Absolute stereochemistry. Rotation (+).

L10 ANSWER 65 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 188566-34-9 CAPLUS
CN Benzenemethanol, α-[(1S)-2,2,2-trifluoro-1-(methylamino)ethyl]-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 66 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

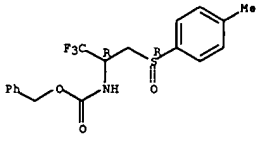
AB In the Experimental Section, most signs of the [α]20D values of the compds. described are missing. The following compds. have pos. (+) [α]20D values: (Z)-3b, (E)-3b, (Z)-3e, (Z)-4a, 9b (both diastereoisomers), 10a (both diastereoisomers), 11a (both diastereoisomers), 12 (both diastereoisomers), (2S,RS)-14, (2S,RS)-15a, (2S,RS)-15c, (S)-16, (R)-17, (R)-19, (R)-21, (R)-22, and (R)-24. The following compds. have neg. (-) [α]20D values: (Z)-3a, (Z)-3c, (Z)-3d, (Z)-5d, (Z)-6a, (Z)-6b, (Z)-7a, (Z)-7b, (Z)-8a, (Z)-8b, and (R)-18.

ACCESSION NUMBER: 1996:733951 CAPLUS
DOCUMENT NUMBER: 126:89105
TITLE: New versatile fluorinated chiral building blocks: synthesis and reactivity of optically pure α-(fluoroalkyl)-β-sulfinylenamines. [Erratum to document cited in CA125:33255]
AUTHOR(S): Arnone, Alberto; Bravo, Pierfrancesco; Capelli, Silvia; Fronza, Giovanni; Meille, Stefano V.; Zanda, Matteo; Cavicchio, Giancarlo; Crucianelli, Marcello
CORPORATE SOURCE: Dipartimento di Chimica, Politecnico Milano, Milan, I-20133, Italy
SOURCE: Journal of Organic Chemistry (1996), 61(26), 9635
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **169138-03-8P 169138-06-1P 177469-11-3P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines (Erratum))

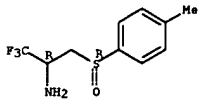
RN 169138-03-8 CAPLUS
CN Carbamic acid, [2,2,2-trifluoro-1-[[(4-methylphenyl)sulfinyl]methyl]ethyl]-, phenylmethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



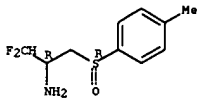
RN 169138-06-1 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



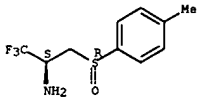
RN 177469-11-3 CAPLUS
CN 2-Propanamine, 1,1-difluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **169138-05-0P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines (Erratum))
RN 169138-05-0 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

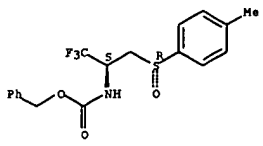
Absolute stereochemistry. Rotation (+).



IT **169138-02-7P 172364-77-1P 177268-09-6P**
**177469-13-5P 177469-14-6P 177469-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines (Erratum))
RN 169138-02-7 CAPLUS
CN Carbamic acid, [2,2,2-trifluoro-1-[[(4-methylphenyl)sulfinyl]methyl]ethyl]-, phenylmethyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

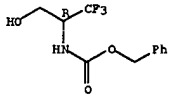
Absolute stereochemistry.





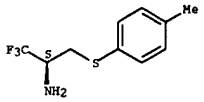
RN 172364-77-1 CAPLUS
CN Carbamic acid, [(1R)-2,2,2-trifluoro-1-(hydroxymethyl)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



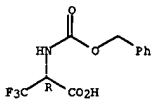
RN 177268-09-6 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(4-methylphenyl)thio]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177469-13-5 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

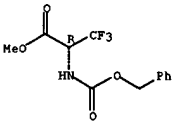
Absolute stereochemistry. Rotation (-).



RN 177469-14-6 CAPLUS

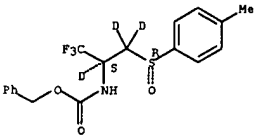

CN L-Alanine, 3,3,3-trifluoro-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



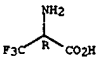
RN 177469-17-9 CAPLUS
CN Carbamic acid, [2-[(4-methylphenyl)sulfinyl]-1-(trifluoromethyl)ethyl-1,2,2-d3]-, phenylmethyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **127127-25-7P 172364-73-7P 172490-05-0P**
**177268-08-5P 177268-13-2P 177268-14-3P**
**177469-12-4P 177469-15-7P 177469-16-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines (Erratum))
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

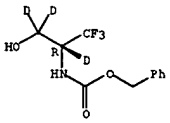
Absolute stereochemistry. Rotation (+).



RN 172364-73-7 CAPLUS
CN Carbamic acid, [2-hydroxy-1-(trifluoromethyl)ethyl-1,2,2-d3]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

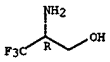
Absolute stereochemistry.





RN 172490-05-0 CAPLUS
CN 1-Propanol, 2-amino-3,3,3-trifluoro-, hydrochloride, (R)- (9CI) (CA INDEX NAME)

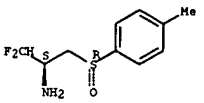
Absolute stereochemistry.



● HCl

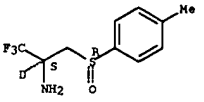
RN 177268-08-5 CAPLUS
CN 2-Propanamine, 1,1-difluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177268-13-2 CAPLUS
CN 2-Propan-2-d-amine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

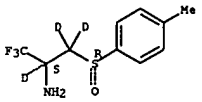
Absolute stereochemistry.



RN 177268-14-3 CAPLUS
CN 2-Propan-1,1,2-d3-amine, 3,3,3-trifluoro-1-[(4-methylphenyl)sulfinyl]-,

{R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



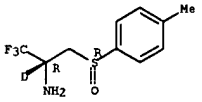
RN 177469-12-4 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

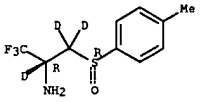
RN 177469-15-7 CAPLUS
CN 2-Propan-2-d-amine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

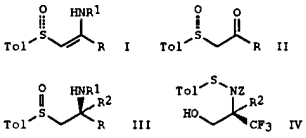


RN 177469-16-8 CAPLUS
CN 2-Propan-1,1,2-d3-amine, 3,3,3-trifluoro-1-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




GI



AB Efficient synthesis of optically pure α-(fluoroalkyl)-β-sulfinyl enamines I [Tol = 4-MeC6H4; R = CF3, CF2H, CF2Cl, CF2CF3, CFH2; R1 = H, CO2CH2Ph (Z)] has been achieved by aza-Wittig reaction of triphenyliminophosphoranes Ph2P:NR1 (R1 = Z, H, SiMe3) with the corresponding α-fluorinated-α'-sulfinyl ketones II. I showed an overwhelming preference for the Z stereochem. of the enamine form. Their general reactivity has been studied. The reaction with some electrophiles (i.e. benzyl chloroformate and benzyl and allyl bromide) occurs at the nitrogen atom providing the corresponding N,N-disubstituted enamines. Nucleophiles add smoothly to C-2: heteroatom-centered nucleophiles like methanol, ammonia, and thiophenol afford gem-disubstituted derivs. under thermodn. control, while a C-centered nucleophile like nitromethane adds in irreversible fashion. The hydride- and deuteride-promoted reduction of I to α-fluorinated-α'-sulfinyl amines III (R2 = H, D) has been studied. Hydride addition was stereoselective, while low stereoselection was obtained with the other tested nucleophiles. Desulfurization of optically pure sulfinylamine III (R = CF3, R1 = R2 = H) afforded (R)-1-(trifluoromethyl)ethylamine. The Pummerer rearrangement of III (R = CF3, R1 = Z) occurs in an unusual nonoxidative way affording sulfenamides IV, that readily provided (R)-3,3,3-trifluoroalaninol and its 2-deutero analog, and (R)-3,3,3-trifluoroalanine.

ACCESSION NUMBER: 1996:259705 CAPLUS
DOCUMENT NUMBER: 125:33255
TITLE: New Versatile Fluorinated Chiral Building Blocks: Synthesis and Reactivity of Optically Pure α-(Fluoroalkyl)-β-sulfinylenamines
AUTHOR(S): Arnone, Alberto; Bravo, Pierfrancesco; Capelli, Silvia; Fronza, Giovanni; Meille, Stefano V.; Zanda, Matteo; Cavicchio, Giancarlo; Crucianelli, Marcello
CORPORATE SOURCE: Dipartimento di Chimica, Politecnico Milano, Milan, I-20133, Italy
SOURCE: Journal of Organic Chemistry (1996), 61(10), 3375-87
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:33255

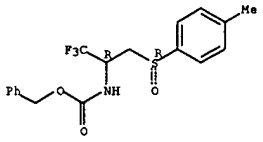
IT **169138-03-8P 169138-06-1P 177469-11-3P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines)

RN 169138-03-8 CAPLUS
CN Carbamic acid, [2,2,2-trifluoro-1-[[(4-methylphenyl)sulfinyl]methyl]ethyl]-



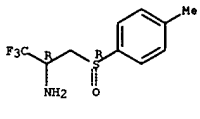

, phenylmethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



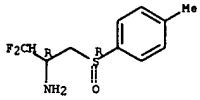
RN 169138-06-1 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177469-11-3 CAPLUS
CN 2-Propanamine, 1,1-difluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

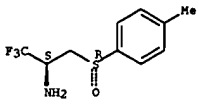
Absolute stereochemistry.



IT **169138-05-0P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines)

RN 169138-05-0 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(R)-(4-methylphenyl)sulfinyl]-, (2S)- (9CI) (CA INDEX NAME)

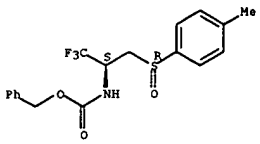
Absolute stereochemistry. Rotation (+).



IT **169138-02-7P 172364-77-1P 177268-09-6P**
**177469-13-5P 177469-14-6P 177469-17-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines)

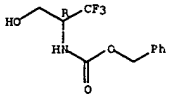
RN 169138-02-7 CAPLUS
CN Carbamic acid, [2,2,2-trifluoro-1-[[(4-methylphenyl)sulfinyl]methyl]ethyl]-, phenylmethyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 172364-77-1 CAPLUS
CN Carbamic acid, [(1R)-2,2,2-trifluoro-1-(hydroxymethyl)ethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

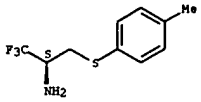
Absolute stereochemistry. Rotation (-).



RN 177268-09-6 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-3-[(4-methylphenyl)thio]-, (S)- (9CI) (CA INDEX NAME)

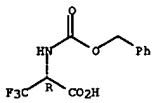
Absolute stereochemistry.





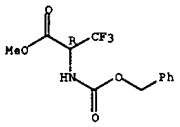
RN 177469-13-5 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



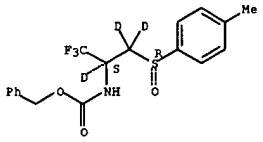
RN 177469-14-6 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177469-17-9 CAPLUS
CN Carbamic acid, [2-[(4-methylphenyl)sulfinyl]-1-(trifluoromethyl)ethyl-1,2,2-d3]-, phenylmethyl ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

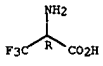




IT **127127-25-7P 172364-73-7P 172490-05-0P**
**177268-08-5P 177268-13-2P 177268-14-3P**
**177469-12-4P 177469-15-7P 177469-16-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of chiral (fluoroalkyl)sulfinylenamines)

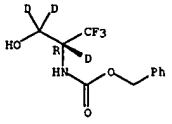
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



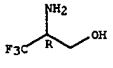
RN 172364-73-7 CAPLUS
CN Carbamic acid, [2-hydroxy-1-(trifluoromethyl)ethyl-1,2,2-d3]-, phenylmethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 172490-05-0 CAPLUS
CN 1-Propanol, 2-amino-3,3,3-trifluoro-, hydrochloride, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

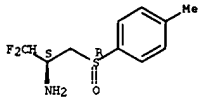


● HCl

RN 177268-08-5 CAPLUS
CN 2-Propanamine, 1,1-difluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

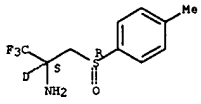
Absolute stereochemistry.





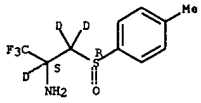
RN 177268-13-2 CAPLUS
CN 2-Propan-2-d-amine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177268-14-3 CAPLUS
CN 2-Propan-1,1,2-d3-amine, 3,3,3-trifluoro-1-[(4-methylphenyl)sulfinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 177469-12-4 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-, hydrochloride, (2R)- (9CI) (CA INDEX NAME)

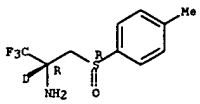
Absolute stereochemistry. Rotation (-).

● HCl

RN 177469-15-7 CAPLUS
CN 2-Propan-2-d-amine, 1,1,1-trifluoro-3-[(4-methylphenyl)sulfinyl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

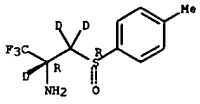
L10 ANSWER 67 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.

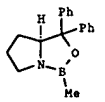


RN 177469-16-8 CAPLUS
CN 2-Propan-1,1,2-d3-amine, 3,3,3-trifluoro-1-[(4-methylphenyl)sulfinyl]-, (R-(R*,R*))- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI

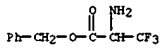


AB Enantiomerically enriched (R)-3,3,3-trifluoroalanine (I) (up to 62% enantiomeric excess) has been synthesized by the asym. reduction of 2-(N-arylimino)-3,3,3-trifluoropropanoic acid esters R1N:C(CF3)CO2R (R = Et, CH2Ph, l-menthyl; R1 = 2,6-Me2C6H3, 3-ClC6H4, Ph, 4-MeC6H4, 4-MeOC6H4) with catecholborane and chiral oxazaborolidine catalyst II and subsequent oxidative removal of N-aromatic moiety with retention of the configuration. Detailed optimization studies revealed that the effects of solvents, temperature, and the structural modification of the substrate were drastic on the enantioselectivity. The absolute configuration of I was determined by x-ray crystallog. of the corresponding N-(S)-(+)-camphorsulfonyl derivative

ACCESSION NUMBER: 1995:1003912 CAPLUS
DOCUMENT NUMBER: 124:202972
TITLE: Asymmetric reduction of 2-(N-arylimino)-3,3,3-trifluoropropanoic acid esters leading to enantiomerically enriched 3,3,3-trifluoroalanine
AUTHOR(S): Sakai, Takashi; Yan, Fengyang; Kashino, Setsuo; Uneyama, Kenji
CORPORATE SOURCE: Fac. Eng., Okayama Univ., Okayama, 700, Japan
SOURCE: Tetrahedron (1996), 52(1), 233-44
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:202972

IT **174075-89-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. reduction of (arylimino)trifluoropropanoates to trifluoroalanines with chiral boron hydrides and catalysts)

RN 174075-89-9 CAPLUS
CN Alanine, 3,3,3-trifluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

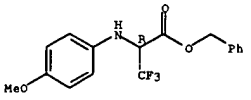


IT **170883-29-1P 170883-32-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. reduction of (arylimino)trifluoropropanoates to trifluoroalanines with chiral boron hydrides and catalysts)

RN 170883-29-1 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, phenylmethyl ester (9CI)

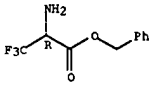
L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170883-32-6 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

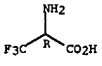
Absolute stereochemistry.



IT **127127-25-7P 170883-25-7P 170883-26-8P**
**170883-27-9P 170883-28-0P 170883-30-4P**
**170883-33-7P 171034-34-7P 174075-83-3P**
**174075-84-4P 174075-85-5P 174075-86-6P**
**174075-87-7P 174075-88-8P 174075-90-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. reduction of (arylimino)trifluoropropanoates to trifluoroalanines with chiral boron hydrides and catalysts)

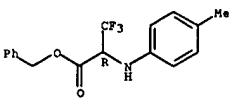
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 170883-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methylphenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

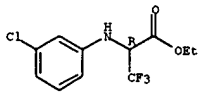
Absolute stereochemistry. Rotation (+).



L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

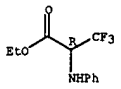
RN 170883-26-8 CAPLUS
CN L-Alanine, N-(3-chlorophenyl)-3,3,3-trifluoro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



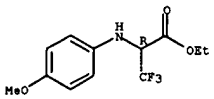
RN 170883-27-9 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



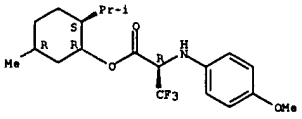
RN 170883-28-0 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170883-30-4 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, [1R-(1α,2β,5α)]- (9CI) (CA INDEX NAME)

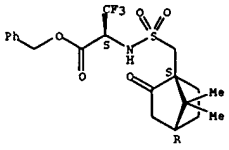
Absolute stereochemistry.



L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

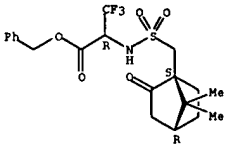
RN 170883-33-7 CAPLUS
CN L-Alanine, N-[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-3,3,3-trifluoro-, phenylmethyl ester, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



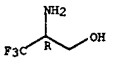
RN 171034-34-7 CAPLUS
CN D-Alanine, N-[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-3,3,3-trifluoro-, phenylmethyl ester, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174075-83-3 CAPLUS
CN 1-Propanol, 2-amino-3,3,3-trifluoro-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

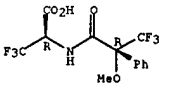


RN 174075-84-4 CAPLUS
CN 1-Propanol, 3,3,3-trifluoro-2-[(4-methoxyphenyl)amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

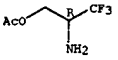
L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.

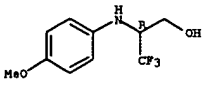


RN 174075-90-2 CAPLUS
CN 1-Propanol, 2-amino-3,3,3-trifluoro-, acetate (ester), (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

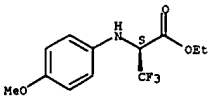


L10 ANSWER 68 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



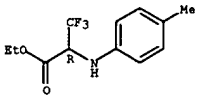
RN 174075-85-5 CAPLUS
CN D-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



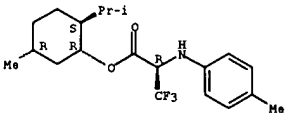
RN 174075-86-6 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methylphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174075-87-7 CAPLUS
CN D-Alanine, 3,3,3-trifluoro-N-(4-methylphenyl)-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, [1R-(1α,2β,5α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 174075-88-8 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(3,3,3-trifluoro-2-methoxy-1-oxo-2-phenylpropyl)-, (R)- (9CI) (CA INDEX NAME)

L10 ANSWER 69 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

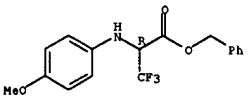
AB (R)-3,3,3-trifluoroalanine and its derivs. have been synthesized enantioselectively by the asym. reduction of 2-(N-arylimino)-3,3,3-trifluoropropanoic acid esters with (S)-oxazaborolidine-catecholborane system. The absolute configuration was determined to be R by X-ray crystallog. anal. of the corresponding N-(S)-(+)-camphorsulfonyl derivative

| | |
|---|---|
| ACCESSION NUMBER: | 1995:761286 CAPLUS |
| DOCUMENT NUMBER: | 124:9362 |
| TITLE: | Asymmetric reduction of 2-(N-arylimino)-3,3,3-trifluoropropanoic acid esters leading to chiral 3,3,3-trifluoroalanine and its derivatives |
| AUTHOR(S): | Sakai, Takashi; Yan, Fengyang; Uneyama, Kenji |
| CORPORATE SOURCE: | Fac. Engineering, Okayama Univ., Okayama, 700, Japan |
| SOURCE: | Synlett (1995), (7), 753-4<br>CODEN: SYNLES; ISSN: 0936-5214 |
| PUBLISHER: | Thieme |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |
| OTHER SOURCE(S): | CASREACT 124:9362 |

IT **170883-29-1P 170883-32-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. reduction of (arylimino)trifluoropropanoates leading to chiral trifluoroalanine and its derivs.)

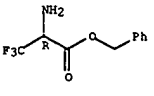
RN 170883-29-1 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170883-32-6 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

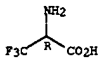
Absolute stereochemistry.



IT **127127-25-7P 170883-25-7P 170883-26-8P 170883-27-9P 170883-28-0P 170883-30-4P 170883-31-5P 170883-33-7P 171034-34-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. reduction of (arylimino)trifluoropropanoates leading to chiral trifluoroalanine and its derivs.)

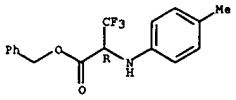
L10 ANSWER 69 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



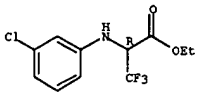
RN 170883-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methylphenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



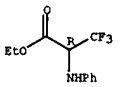
RN 170883-26-8 CAPLUS
CN L-Alanine, N-(3-chlorophenyl)-3,3,3-trifluoro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 170883-27-9 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

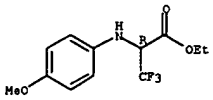
Absolute stereochemistry. Rotation (-).



RN 170883-28-0 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

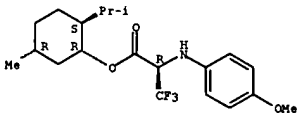
Absolute stereochemistry. Rotation (-).

L10 ANSWER 69 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

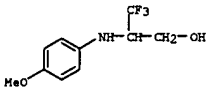


RN 170883-30-4 CAPLUS
CN L-Alanine, 3,3,3-trifluoro-N-(4-methoxyphenyl)-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, [1R-(1α,2β,5α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

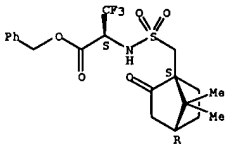


RN 170883-31-5 CAPLUS
CN 1-Propanol, 3,3,3-trifluoro-2-[(4-methoxyphenyl)amino]- (9CI) (CA INDEX NAME)



RN 170883-33-7 CAPLUS
CN L-Alanine, N-[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-3,3,3-trifluoro-, phenylmethyl ester, (1S)- (9CI) (CA INDEX NAME)

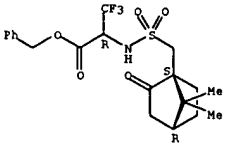
Absolute stereochemistry.



RN 171034-34-7 CAPLUS
CN D-Alanine, N-[[(7,7-dimethyl-2-oxobicyclo[2.2.1]hept-1-yl)methyl]sulfonyl]-

L10 ANSWER 69 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
3,3,3-trifluoro-, phenylmethyl ester, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L10 ANSWER 70 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB This work explores the biomimetic potential of [18F]fluorine for hydroxy substitution in β-phenethanolamines as a possible strategy for developing radiotracers for in vivo imaging. Stereospecific syntheses of the two model compds. (1R,2S)-1-[18F]fluoro-1-deoxyephedrine ([18F]FDE) and (1S,2S)-1-[18F]fluoro-1-deoxypseudoephedrine ([18F]FDP) were achieved in high radiochem. yield (62%, decay corrected) and high specific activity (>2500 Ci/mmol) by reaction of [18F]fluoride ion with the appropriate chiral cyclic sulfamidate precursor. Both tracers exhibited good stability toward metabolic defluorination in vivo. High, homogeneous brain uptake (.apprx.8% of injected dose) was observed after i.v. injection in mice similar to that reported for the structurally related analog [11C]methamphetamine. The 1R,2S isomer (FDE) showed a 3-fold higher concentration of radioactivity in whole brain as compared to the 1S,2S isomer (FDP). These results suggest possible employment of this strategy for chiral radiolabeling of biol. important phenethanolamines and catecholamines.

| | |
|---|---|
| ACCESSION NUMBER: | 1995:380747 CAPLUS |
| DOCUMENT NUMBER: | 122:182135 |
| TITLE: | Fluorine for Hydroxy Substitution in Biogenic Amines: Asymmetric Synthesis and Biological Evaluation of Fluorine-18-Labeled β-Fluorophenylalkylamines as Model Systems |
| AUTHOR(S): | Van Dort, Marcian E.; Jung, Yong-Woon; Sherman, Philip S.; Kilbourn, Michael R.; Wieland, Donald M. |
| CORPORATE SOURCE: | Medical School, University of Michigan, Ann Arbor, MI, 48109-0552, USA |
| SOURCE: | Journal of Medicinal Chemistry (1995), 38(5), 810-15 CODEN: JMCMAR; ISSN: 0022-2623 |
| PUBLISHER: | American Chemical Society |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |

IT **161403-39-0P 161403-40-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
([18F]fluorophenylalkylamines preparation and biodistribution for PET)

RN 161403-39-0 CAPLUS
CN Benzeneethanamine, β-(fluoro-18F)-N,α-dimethyl-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 161403-40-3 CAPLUS
CN Benzeneethanamine, β-(fluoro-18F)-N,α-dimethyl-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 70 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT 64068-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
([18F]fluorophenylalkylamines preparation and biodistribution for PET)
RN 64068-21-9 CAPLUS
CN Benzeneethanamine, β-fluoro-N,α-dimethyl-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

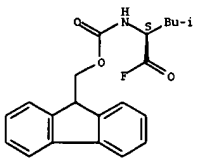
Absolute stereochemistry.

● HCl

L10 ANSWER 71 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB The standard methods of stepwise solid phase synthesis according to Merrifield could not previously be applied to the synthesis of the important naturally occurring peptaibols because of difficulties arising from the pronounced steric hindrance caused by α,α-dialkylated amino acids (incomplete coupling, especially to adjacent similarly constituted units, racemization due to slow coupling to hindered amino acids, etc.), chain degradation due to the presence of acid-labile Aib-Pro (Aib = α-aminoisobutyric acid) linkages, and the lack of any general method for the loading of C-terminal amino alcs. to resin supports. Following recent work on model systems, it is now shown that the adoption of 9-fluorenylmethoxycarbonyl (Fmoc) amino acid fluorides as coupling reagents makes possible the facile, general assembly of such peptides. The method was demonstrated for alamethicin F30 and F50, saturnisporin SA III, and trichotoxin A50-J. The crude products were of remarkable purity. Amino acid anal., mass spectral data, and comparison of the synthetic alamethicins with samples of naturally occurring material confirmed the success of the syntheses. No significant amount of racemization (<0.8%) was found for any of the chiral amino acids present. The first step of the synthesis involved a new general method for assembly of C-terminal peptide alcs. via the use of o-chlorotrityl resin. In addition, model studies on the question of racemization during the coupling of Fmoc amino acid fluorides are reported.
ACCESSION NUMBER: 1995:308989 CAPLUS
DOCUMENT NUMBER: 122:133824
TITLE: Stepwise Automated Solid Phase Synthesis of Naturally Occurring Peptaibols Using FMOC Amino Acid Fluorides
AUTHOR(S): Wenschuh, Holger; Beyermann, Michael; Haber, Hanka; Seydel, Joachim K.; Krause, Eberhard; Bienert, Michael; Carpino, Louis A.; El-Faham, Ayman; Albericio, Fernando
CORPORATE SOURCE: Institute of Molecular Pharmacology, Berlin, D-10315, Germany
SOURCE: Journal of Organic Chemistry (1995), 60(2), 405-10
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 130858-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(stepwise automated solid phase synthesis of naturally occurring peptaibols using fluorenylmethoxycarbonylamino acid fluorides)
RN 130858-94-5 CAPLUS
CN Carbamic acid, [(1S)-1-(fluorocarbonyl)-3-methylbutyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)

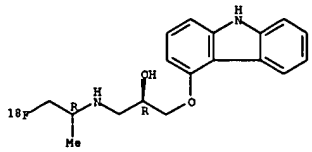
Absolute stereochemistry.

L10 ANSWER 71 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L10 ANSWER 72 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB New β-adrenergic receptor antagonists, 2-(R)-(+)- and 2-(S)-(-)-1-(9H-carbazol-4-yl-oxy)-3-[[1-(fluoromethyl)ethyl]amino]-2-propanol ((S)- and (R)-fluorocarazolols), were labeled with fluorine-18 at the no-carrier-added level by reductive alkylation of desisopropylcarazolol (4-(2-hydroxy-3-amino-1-propoxy)carbazole) with [18F]fluoroacetone. The latter was prepared by nucleophilic substitution of fluoride on acetol tosylate and may serve as a useful synthetic precursor for other radiotracers. The radiochem. yield of [18F]fluorocarazolol (500-1200Ci/mmol) from [18F]fluoride was 40% at the end of the 45 min synthesis. Chiral HPLC showed >99% enantiomeric purity of 2-(S)- and 2-(R)-[18F]fluorocarazolols. The log P of fluorocarazolol was 2.2 at pH 7.4. The in vitro KD values of (S)- and (R)-fluorocarazolol for the β-adrenergic receptor were measured in a rat heart preparation to be KD = 68 and 1128 pM, resp. Biodistribution expts. in mice demonstrated specific β-adrenergic receptor binding of (S)-[18F]fluorocarazolol. (R)-[18F]fluorocarazolol showed no observable specific binding to β-receptors in vivo. The uptake of (R)-[18F]fluorocarazolol may therefore be used as an estimation of nonspecific binding. Positron emission tomog. images of pigs showed receptor-specific uptake of (S)-[18F]fluorocarazolol in the heart and lung. Washout of dissociated ligand from the tissue was observed only after 70 min postinjection. The maximum ratio of specific to nonspecific uptake in pig heart and lung was .apprx.10 at 150 min postinjection. Observed levels of fluorocarazolol metabolites in mouse and pig blood were relatively low and remained fairly constant during the period from 10 to 180 min postinjection. These results indicate that (S)-(-)-[18F]fluorocarazolol is of interest for use as a radiopharmaceutical for estimation of β-adrenergic receptors with positron tomog.
ACCESSION NUMBER: 1994:596101 CAPLUS
DOCUMENT NUMBER: 121:196101
TITLE: Synthesis, Binding Properties, and 18F Labeling of Fluorocarazolol, a High-Affinity β-Adrenergic Receptor Antagonist
AUTHOR(S): Zheng, Lei; Berridge, Marc S.; Ernsberger, Paul
CORPORATE SOURCE: School of Medicine, Case Western Reserve University, Cleveland, OH, USA
SOURCE: Journal of Medicinal Chemistry (1994), 37(20), 3219-30
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157989-08-7P 157989-09-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 157989-08-7 CAPLUS
CN 2-Propanol, 1-(9H-carbazol-4-yloxy)-3-[[2-(fluoro-18F)-1-methylethyl]amino]-, monohydrochloride, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

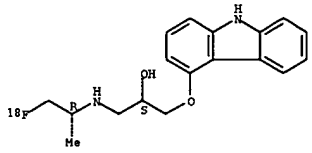
Absolute stereochemistry.



● HCl

RN 157989-09-8 CAPLUS
CN 2-Propanol, 1-(9H-carbazol-4-yloxy)-3-[[2-(fluoro-18F)-1-methylethyl]amino]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

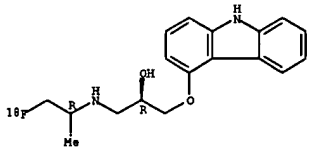


● HCl

IT **157989-10-1P 157989-11-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, β-adrenergic receptors determination by positron emission tomog. in relation to)
RN 157989-10-1 CAPLUS
CN 2-Propanol, 1-(9H-carbazol-4-yloxy)-3-[[2-(fluoro-18F)-1-methylethyl]amino]-, (R-(R*,R*))- (9CI) (CA INDEX NAME)

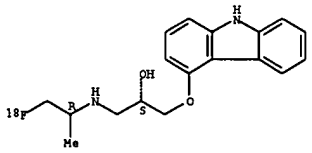
Absolute stereochemistry.



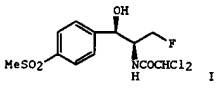


RN 157989-11-2 CAPLUS
CN 2-Propanol, 1-(9H-carbazol-4-yloxy)-3-[[(1R)-2-(fluoro-18F)-1-methylethyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




GI



I

AB The present invention comprises a process for the asym. synthesis of florfenicol, I, thiamphenicol, or chloramphenicol. The S,S isomer of florfenicol is isomerized to the R,S isomer by sequentially treating with: (i) a lower alkylsulfonyl chloride and a tertiary amine base; (ii) sulfuric acid and water; and (iii) an alkali metal hydroxide. The present invention further comprises a process for regioselectively opening an epoxide to form a threo-oxazoline.

ACCESSION NUMBER: 1994:533722 CAPLUS
DOCUMENT NUMBER: 121:133722
TITLE: Asymmetric process for preparing florfenicol, thiamphenicol, chloramphenicol and oxazoline intermediates
INVENTOR(S): Wu, Guang-Zhong; Tormos, Wanda I.
PATENT ASSIGNEE(S): Schering Corp., USA
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

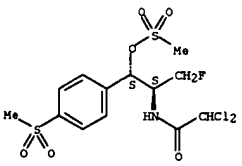
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9414764 | A1 | 19940707 | WO 1993-US12071 | 19931215 |
| W: AU, BB, BG, BR, BY, CA, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| US 5352832 | A | 19941004 | US 1992-993932 | 19921218 |
| CA 2152089 | AA | 19940707 | CA 1993-2152089 | 19931215 |
| AU 9457484 | A1 | 19940719 | AU 1994-57484 | 19931215 |
| AU 676003 | B2 | 19970227 | | |
| EP 674618 | A1 | 19951004 | EP 1994-903599 | 19931215 |
| EP 674618 | B1 | 19980909 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| HU 72669 | A2 | 19960528 | HU 1995-1776 | 19931215 |
| JP 08504819 | T2 | 19960528 | JP 1994-515232 | 19931215 |
| JP 3428016 | B2 | 20030722 | | |
| AT 170835 | E | 19980915 | AT 1994-903599 | 19931215 |
| ES 2120605 | T3 | 19981101 | ES 1994-903599 | 19931215 |
| RU 2126383 | C1 | 19990220 | RU 1995-115555 | 19931215 |
| PL 177891 | B1 | 20000131 | PL 1993-309393 | 19931215 |
| CZ 287461 | B6 | 20001115 | CZ 1995-1598 | 19931215 |
| SK 281701 | B6 | 20010710 | SK 1995-777 | 19931215 |
| FI 9502872 | A | 19950612 | FI 1995-2872 | 19950612 |
| FI 109295 | B1 | 20020628 | | |
| NO 9502425 | A | 19950616 | NO 1995-2425 | 19950616 |



PRIORITY APPLN. INFO.: US 1992-993932 A 19921218
WO 1993-US12071 W 19931215
OTHER SOURCE(S): CASREACT 121:133722; MARPAT 121:133722

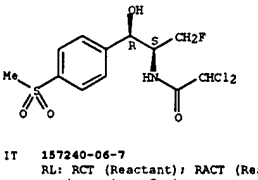
IT **157142-65-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of fluorfenicol)
RN 157142-65-9 CAPLUS
CN Acetamide, 2,2-dichloro-N-[1-(fluoromethyl)-2-[(methylsulfonyl)oxy]-2-[4-(methylsulfonyl)phenyl]ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



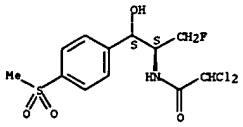
IT **73231-34-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from asym. starting materials)
RN 73231-34-2 CAPLUS
CN Acetamide, 2,2-dichloro-N-[(1S,2R)-1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **157240-06-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of fluorfenicol)
RN 157240-06-7 CAPLUS
CN Acetamide, 2,2-dichloro-N-[1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





AB The monofluorinated analogs of 2-aminocarboxylic acids up to C7 were efficiently separated into the diastereomers on glass capillary columns coated with achiral phases BP-1, BP-10 and OV-330. In addition, some difluoro and trifluoro analogs were also measured. Chiral resolution was achieved on capillary wall-coated open tubular fused-silica columns coated with chiral phases XE-60-L-Val-L-(1-phenylethyl)amide, Chirasil-L-Val and Behenoyl-L-Val-tert-butylamide. The separation factors and the Kovats indexes of the fluorinated amino acids were determined and compared.

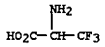
The erythro racemates display a higher degree of resolution than the threo ones. The order of elution was found to be the L- after the D-solute on all L-phases.

ACCESSION NUMBER: 1994:123831 CAPLUS
DOCUMENT NUMBER: 120:123831
TITLE: Gas chromatographic separation of diastereoisomeric and enantiomeric forms of some fluorinated amino acids on glass capillary columns
AUTHOR(S): Vlasakova, V.; Tolman, V.; Zivny, K.
CORPORATE SOURCE: Institute of Nuclear Biology and Radiochemistry, Czech Academy of Sciences, Videnska 1083, Prague, 14220/4, Czech.
SOURCE: Journal of Chromatography (1993), 639(2), 273-9
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **16652-37-2 17463-43-3 43163-94-6 84277-05-4 84277-08-7 110415-69-5 110415-70-8 110415-71-9 110415-72-0 149560-55-4 149560-58-7**
RL: ANST (Analytical study); PROC (Process)
(resolution of, by capillary gas chromatog.)

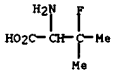
RN 16652-37-2 CAPLUS
CN Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)



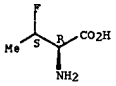
RN 43163-94-6 CAPLUS
CN Valine, 3-fluoro- (9CI) (CA INDEX NAME)





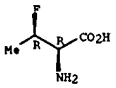
RN 84277-05-4 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



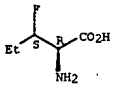
RN 84277-08-7 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



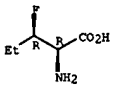
RN 110415-69-5 CAPLUS
CN Norvaline, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 110415-70-8 CAPLUS
CN Norvaline, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

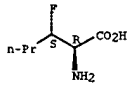
Relative stereochemistry.





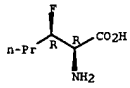
RN 110415-71-9 CAPLUS
CN Norleucine, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

Relative stereochemistry.



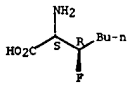
RN 110415-72-0 CAPLUS
CN Norleucine, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



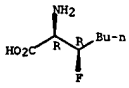
RN 149560-55-4 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 149560-58-7 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, (R*,R*)- (9CI) (CA INDEX NAME)

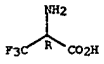
Relative stereochemistry.



IT **127127-25-7 129939-36-2**
RL: ANST (Analytical study); PROC (Process)
(separation of, from enantiomer)

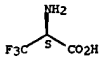
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



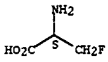
RN 129939-36-2 CAPLUS
CN D-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



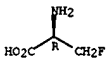
IT 35455-20-0 35455-21-1 58960-35-3
59752-74-8 64813-63-4 68781-14-6
68781-15-7 68781-16-8 149560-44-1
149560-45-2 149560-47-4 149560-48-5
149560-50-9 149560-51-0 149560-53-2
149560-54-3 149560-56-5 149560-57-6
149560-59-8 149560-60-1
RL: ANT (Analyte); ANST (Analytical study)
(separation of, from enantiomer by capillary gas chromatog.)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

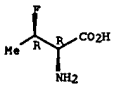
Absolute stereochemistry.



RN 58960-35-3 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

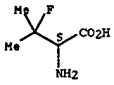
Absolute stereochemistry.





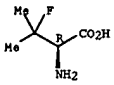
RN 59752-74-8 CAPLUS
CN D-Valine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



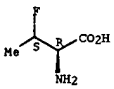
RN 64813-63-4 CAPLUS
CN L-Valine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 68781-14-6 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, (S-(R*,S*))- (9CI) (CA INDEX NAME)

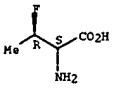
Absolute stereochemistry.



RN 68781-15-7 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

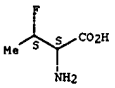
Absolute stereochemistry.





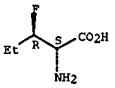
RN 68781-16-8 CAPLUS
CN Butanoic acid, 2-amino-3-fluoro-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



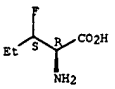
RN 149560-44-1 CAPLUS
CN D-Norvaline, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149560-45-2 CAPLUS
CN L-Norvaline, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

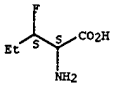
Absolute stereochemistry.



RN 149560-47-4 CAPLUS
CN D-Norvaline, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

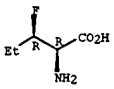
Absolute stereochemistry.





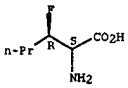
RN 149560-48-5 CAPLUS
CN L-Norvaline, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



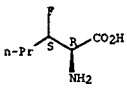
RN 149560-50-9 CAPLUS
CN D-Norleucine, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



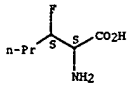
RN 149560-51-0 CAPLUS
CN L-Norleucine, 3-fluoro-, erythro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



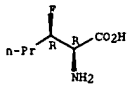
RN 149560-53-2 CAPLUS
CN D-Norleucine, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



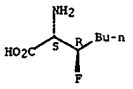
RN 149560-54-3 CAPLUS
CN L-Norleucine, 3-fluoro-, threo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



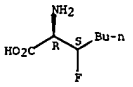
RN 149560-56-5 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149560-57-6 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

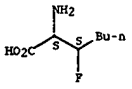
Absolute stereochemistry.



RN 149560-59-8 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

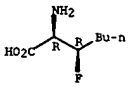
Absolute stereochemistry.





RN 149560-60-1 CAPLUS
CN Heptanoic acid, 2-amino-3-fluoro-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



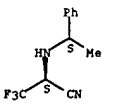
L10 ANSWER 75 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB CF3CH(CN)NHR [I; R = branched or cyclic (heteroatom- or double bond-containing) chiral alkyl] are prepared by treating CF3CH:NR (II; R = same as I) with metal cyanides. Optically active II (R = CHMePH) and Me3SiCN in CH2Cl2 were treated with ZnI2 at 0° overnight to give 71% 2:1 diastereomeric mixture of I (R = CHMePh).

ACCESSION NUMBER: 1993:670645 CAPLUS
DOCUMENT NUMBER: 119:270645
TITLE: Preparation of optically active trifluoroalanine precursors
INVENTOR(S): Kubota, Toshio; Masaki, Futoshi; Katagiri, Toshimasa
PATENT ASSIGNEE(S): Nitsuko Kyoseki Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 05186411 | A2 | 19930727 | JP 1992-20635 | 19920110 |
| PRIORITY APPLN. INFO.: | | | JP 1992-20635 | 19920110 |

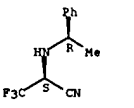
OTHER SOURCE(S): CASREACT 119:270645; MARPAT 119:270645
IT **151331-10-1P 151331-12-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from trifluoroethanimine and trimethylsilyl cyanide)
RN 151331-10-1 CAPLUS
CN Propanenitrile, 3,3,3-trifluoro-2-[(1-phenylethyl)amino]-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



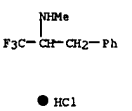
RN 151331-12-3 CAPLUS
CN Propanenitrile, 3,3,3-trifluoro-2-[(1-phenylethyl)amino]-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L10 ANSWER 76 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB In the course of the 1H NMR investigation of selegiline and compds. related to it, the 3J coupling consts. of the protons of the α and the β carbon of the β-phenylethylamine moiety were determined The rotamer populations around the single bond of the α and β C were calculated from these values. The effects of substituents on the α-C atom, the N atom and on the Ph ring, as well as the solvent on the conformational equilibrium were determined The optical purity of the samples was determined using chiral Eu-shift reagents. The coordination process between p-fluoroamphetamine and Eu(tcf)3 was studied in detail, the formation constant of the complex and the chemical shifts were determined

ACCESSION NUMBER: 1993:524981 CAPLUS
DOCUMENT NUMBER: 119:124981
TITLE: NMR investigation of selegiline and compounds related to it
AUTHOR(S): Podanyi, Benjamin
CORPORATE SOURCE: Chinoin Gyogyszer Vegyeszeti Termekek Gyara Rt., Budapest, Hung.
SOURCE: Acta Pharmaceutica Hungarica (1992), 62(5), 218-24
CODEN: APHGAO; ISSN: 0001-6659
DOCUMENT TYPE: Journal
LANGUAGE: Hungarian
IT **149225-51-4**
RL: PRP (Properties)
(NMR spectroscopy of)
RN 149225-51-4 CAPLUS
CN Benzeneethanamine, N-methyl-α-(trifluoromethyl)-, hydrochloride (9CI) (CA INDEX NAME)



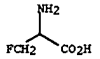
L10 ANSWER 77 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

AB The separation of enantiomers of 3-fluoroalanine, 3,3-difluoroalanine and 3,3,3-trifluoroalanine on ChiralProCu, ChiralValCu and Chiral-1 Nucleosil columns was studied. The substitution of hydrogen for fluorine atoms results in a significant increase in the selectivity of separation of the enantiomers. The relationship between the number of fluorine atoms and the retention of enantiomers on different columns was studied. Optimum conditions for the separation of enantiomers were found.

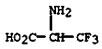
ACCESSION NUMBER: 1992:439544 CAPLUS
DOCUMENT NUMBER: 117:39544
TITLE: High-performance ligand-exchange liquid chromatography of fluoro derivatives of alanine
AUTHOR(S): Galushko, S. V.; Shishkina, I. P.; Gerus, I. I.; Kolycheva, M. T.
CORPORATE SOURCE: Inst. Bioorg. Chem. Oil Chem., Kiev, 253660, Ukraine
SOURCE: Journal of Chromatography (1992), 600(1), 83-5
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **16652-37-2 17463-43-3 109584-01-2**
RL: PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(dissoln. of, by high-performance ligand-exchange liquid chromatog. on chiral stationary phases)

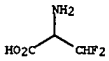
RN 16652-37-2 CAPLUS
CN Alanine, 3-fluoro- (9CI) (CA INDEX NAME)



RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

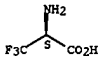


RN 109584-01-2 CAPLUS
CN Alanine, 3,3-difluoro- (9CI) (CA INDEX NAME)



IT **35455-20-0 35455-21-1 59729-23-6 78887-06-6 127127-25-7 129939-36-2**
RL: ANST (Analytical study); PROC (Process)
(separation of, from enantiomer by high-performance ligand-exchanged liquid chromatog. on chiral stationary phases)

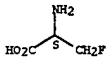
L10 ANSWER 77 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L10 ANSWER 77 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

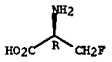
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



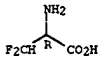
RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



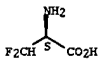
RN 59729-23-6 CAPLUS
CN L-Alanine, 3,3-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



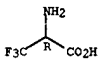
RN 78887-06-6 CAPLUS
CN D-Alanine, 3,3-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

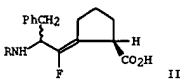


RN 129939-36-2 CAPLUS
CN D-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L10 ANSWER 78 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

GI



II

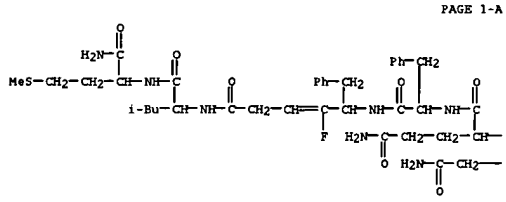
AB A report from a symposium on the preparation of trans-fluoroolefin dipeptide isosteres (E)-RNHCHR1CF:CHCHR2CO2R3 [I; R = Me3O2C (Boc), 9-fluorenylmethoxycarbonyl (Fmoc); R1 = H, CH2Ph; R2 = H, CH2Ph; R3 = OH] and II (R = Boc, Fmoc). I were prepared by several olefination and alkylation reactions, as well as hetero-Cope rearrangements of allylic imino esters to give chiral derivs. I. II were prepared by alkylation and fluoroolefination of cyclopentanone derivs. (S)- And (R)-I (R = Fmoc, R1 = CH2Ph, R2 = H, R3 = OH) were converted into substance P analogs (R)- and (S)-I (R = H-Arg-Pro-Lys-Pro-Gln-Gln-Phe, R1 = CH2Ph, R2 = H, R3 = Leu-Met-NH2), and their binding affinities toward substance P receptors determined

ACCESSION NUMBER: 1991:186051 CAPLUS
DOCUMENT NUMBER: 114:186051
TITLE: Fluoroolefin dipeptide isosteres
AUTHOR(S): Allmendinger, Thomas; Felder, Eduard; Hungerbuehler, Ernst
CORPORATE SOURCE: Cent. Res. Lab., Ciba-Geigy A.-G., Basel, CH-4002, Switz.
SOURCE: ACS Symposium Series (1991), 456(Sel. Fluorination Org. Bioorg. Chem.), 186-95
CODEN: ACSMC8; ISSN: 0097-6156
DOCUMENT TYPE: Journal
LANGUAGE: English

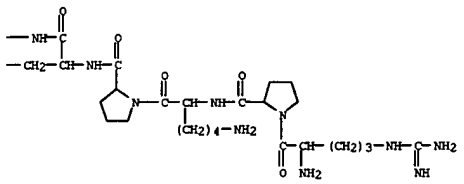
IT **132549-53-2P 132618-90-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and binding of, to substance P receptors)

RN 132549-53-2 CAPLUS
CN Substance P, 8-[(Z)-β,γ-didehydro-γ-fluoro-L-δ-aminobenzenehexanoic acid]-9-deglycine- (9CI) (CA INDEX NAME)

PAGE 1-A

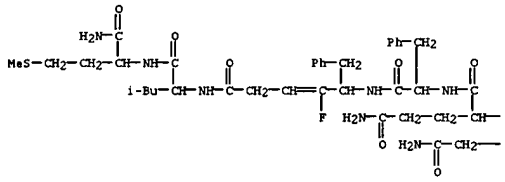


PAGE 1-B



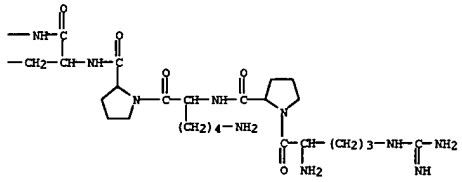
RN 132618-90-7 CAPLUS
CN Substance P, 8-[(Z)-β,γ-didehydro-γ-fluoro-D-δ-aminobenzenehexanoic acid]-9-deglycine- (9CI) (CA INDEX NAME)

PAGE 1-A



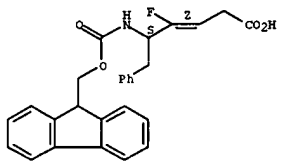


PAGE 1-B



IT **129599-84-4P 129599-85-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and peptide coupling reactions of, substance P analog from)
RN 129599-84-4 CAPLUS
CN 3-Hexenoic acid, 5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, [S-(Z)]- (9CI) (CA INDEX NAME)

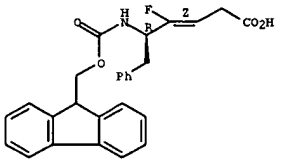
Absolute stereochemistry.
Double bond geometry as shown.



RN 129599-85-5 CAPLUS
CN 3-Hexenoic acid, 5-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, [R-(Z)]- (9CI) (CA INDEX NAME)

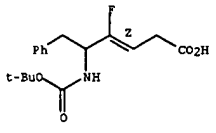
Absolute stereochemistry.
Double bond geometry as shown.



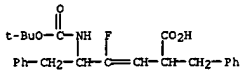


IT **129599-77-5P 129599-78-6P 129599-82-2P**
**129599-86-6P 129599-87-7P 129678-05-3P**
**129704-64-9P 129704-65-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as dipeptide isostere)
RN 129599-77-5 CAPLUS
CN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



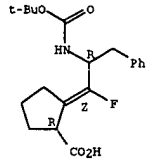
RN 129599-78-6 CAPLUS
CN Benzenepropanoic acid, α-[3-[[(1,1-dimethylethoxy)carbonyl]amino]-2-fluoro-4-phenyl-1-butenyl]- (9CI) (CA INDEX NAME)



RN 129599-82-2 CAPLUS
CN Cyclopentanecarboxylic acid, 2-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-1-fluoro-3-phenylpropylidene]-, [R*,R*-(Z)]- (9CI) (CA INDEX NAME)

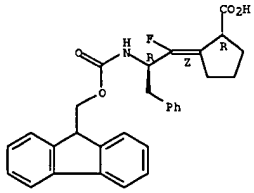
Relative stereochemistry.
Double bond geometry as shown.





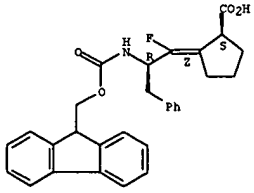
RN 129599-86-6 CAPLUS
CN Cyclopentanecarboxylic acid, 2-[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-fluoro-3-phenylpropylidene]-, [R*,R*-(Z)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



RN 129599-87-7 CAPLUS
CN Cyclopentanecarboxylic acid, 2-[2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-fluoro-3-phenylpropylidene]-, [R*,S*-(Z)]- (9CI) (CA INDEX NAME)

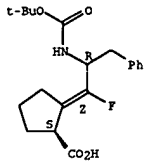
Relative stereochemistry.
Double bond geometry as shown.



L10 ANSWER 78 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

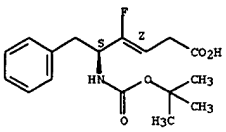
RN 129678-05-3 CAPLUS
CN Cyclopentanecarboxylic acid, 2-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-1-fluoro-3-phenylpropylidene]-, [R*,S*-(Z)]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



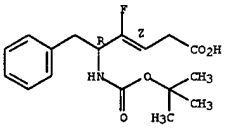
RN 129704-64-9 CAPLUS
CN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, [S-(Z)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 129704-65-0 CAPLUS
CN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-4-fluoro-6-phenyl-, [R-(Z)]- (9CI) (CA INDEX NAME)

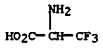
Absolute stereochemistry.
Double bond geometry as shown.



L10 ANSWER 79 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

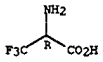
AB The chromatog. behavior of some α-trifluoromethyl-α-amino acids on L-proline and L-hydroxyproline sorbents was studied. The retention and selectivity parameters of the separation of amino acid enantiomers on the sorbents were determined The introduction of a CF group led to an increased selectivity in the separation of amino acid enantiomers on a proline sorbent and to a decreased selectivity on a hydroxyproline sorbent.

ACCESSION NUMBER: 1990:623852 CAPLUS
DOCUMENT NUMBER: 113:223852
TITLE: Ligand-exchange chromatography of α-trifluoromethyl-α-amino acids on chiral sorbents
AUTHOR(S): Galushko, S. V.; Shishkina, I. P.; Soloshonok, V. A.; Kukhar, V. P.
CORPORATE SOURCE: Inst. Bioorg. Chem., Kiev, 252660, USSR
SOURCE: Journal of Chromatography (1990), 511, 115-21
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **17463-43-3**
RL: ANST (Analytical study); PROC (Process)
(resolution of, by ligand-exchange chromatog. on chiral sorbents, attempted)
RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)



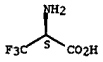
IT **127127-25-7 129939-36-2**
RL: ANST (Analytical study)
(to)
RN 127127-25-7 CAPLUS
CN L-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



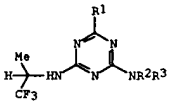
RN 129939-36-2 CAPLUS
CN D-Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L10 ANSWER 79 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L10 ANSWER 80 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI



I

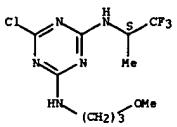
AB L-I [R1 = Cl, F; R2 = H, alkyl; R3 = alkyl, alkoxyalkyl, haloalkyl, alkenyl, (halo)phenylalkyl], were prepared Thus, cyanuric chloride in PhMe at 8-10° was treated with L-MeCH(CF3)NH2 (preparation from L-alanine given) and then aqueous NaOH; after 15-30 min, H2NCH2CH2CH2OMe was added at 15-20° followed by addnl. aqueous NaOH to give 95% L-I [R1 = Cl, R2 = H, R3 = (CH2)3OMe]. Several L-I at 500 g/ha preemergent gave complete control of Abutilon.

ACCESSION NUMBER: 1990:612024 CAPLUS
DOCUMENT NUMBER: 113:212024
TITLE: Preparation of L-2-halo-4-amino-6-(1-methyl-2,2,2-trifluoroethylamino)-s-triazines as herbicides
INVENTOR(S): Tarnow, Horst; Baasner, Bernd; Luerssen, Klaus; Santel, Hans Joachim; Schmidt, Rudolf R.
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

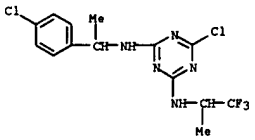
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 3900300 | A1 | 19900712 | DE 1989-3900300 | 19890107 |
| PRIORITY APPLN. INFO.: | | | DE 1989-3900300 | 19890107 |

OTHER SOURCE(S): CASREACT 113:212024; MARPAT 113:212024
IT **130443-77-5P 130443-78-6P 130443-79-7P**
**130443-80-0P 130443-81-1P 130443-82-2P**
**130443-83-3P 130443-84-4P 130443-85-5P**
**130443-86-6P 130443-87-7P 130443-88-8P**
**130443-89-9P 130443-90-2P 130443-91-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 130443-77-5 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(3-methoxypropyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

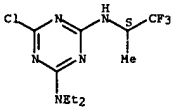


RN 130443-78-6 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-[1-(4-chlorophenyl)ethyl]-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)



RN 130443-79-7 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N,N-diethyl-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

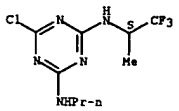
Absolute stereochemistry.



RN 130443-80-0 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-propyl-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

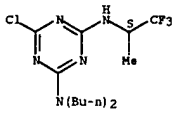
Absolute stereochemistry.





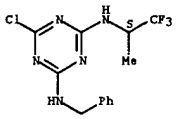
RN 130443-81-1 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, N,N-dibutyl-6-chloro-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 130443-82-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(phenylmethyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

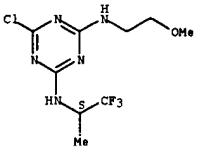
Absolute stereochemistry.



RN 130443-83-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(2-methoxyethyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

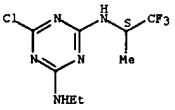
Absolute stereochemistry.





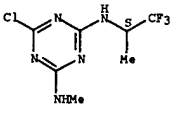
RN 130443-84-4 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 130443-85-5 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-methyl-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

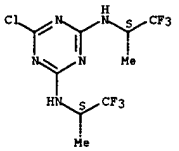
Absolute stereochemistry.



RN 130443-86-6 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-bis(2,2,2-trifluoro-1-methylethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

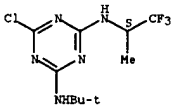
Absolute stereochemistry.





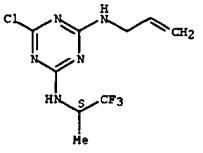
RN 130443-87-7 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylethyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 130443-88-8 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-2-propenyl-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

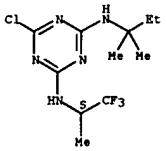
Absolute stereochemistry.



RN 130443-89-9 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1,1-dimethylpropyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

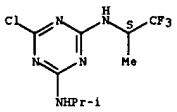
Absolute stereochemistry.

L10 ANSWER 80 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



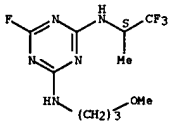
RN 130443-90-2 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-chloro-N-(1-methylethyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 130443-91-3 CAPLUS
CN 1,3,5-Triazine-2,4-diamine, 6-fluoro-N-(3-methoxypropyl)-N'-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

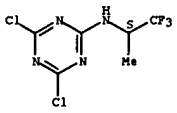
Absolute stereochemistry.



IT **130443-92-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as herbicide intermediate)
RN 130443-92-4 CAPLUS
CN 1,3,5-Triazin-2-amine, 4,6-dichloro-N-(2,2,2-trifluoro-1-methylethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 80 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **125278-10-6P 125353-44-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for triazine herbicide)
RN 125278-10-6 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-, (2S)- (9CI) (CA INDEX NAME)

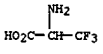
Absolute stereochemistry.

RN 125353-44-8 CAPLUS
CN 2-Propanamine, 1,1,1-trifluoro-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

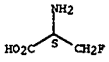
● HCl

L10 ANSWER 81 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB Enantiomers of α-trifluoromethyl-α-amino acids were separated on chiral sorbent containing hydroxyproline residue (Si-100-Polyol-Pro-Gu). The retention of enantiomers depended on the Cu concentration (10-2-10-3M
CuSO4) in the mobile phase. Addition of 30-40% organic solvents (MeOH, EtOH) to
the mobile phase practically did not affect the retention; however, further increase in the concentration in the mobile phase decreased the efficiency. The α-trifluoromethyl group substantially increases the selective separation of amino acid enantiomers.
ACCESSION NUMBER: 1989:111035 CAPLUS
DOCUMENT NUMBER: 110:111035
TITLE: Determination of enantiomeric composition of α-trifluoromethyl-α-amino acids by ligand-exchange microcolumn chromatography
AUTHOR(S): Galushko, S. V.; Shishkina, I. P.; Kobzev, S. P.; Soloshonok, V. A.; Yagupol'skii, Yu. L.; Kukhar, V. P.
CORPORATE SOURCE: Inst. Bioorg. Chem., Kiev, USSR
SOURCE: Zhurnal Analiticheskoi Khimii (1988), 43(11), 2067-9
CODEN: ZAKHA8; ISSN: 0044-4502
DOCUMENT TYPE: Journal
LANGUAGE: Russian
IT **17463-43-3**, Racemic α-trifluoromethylglycine
RL: PROC (Process)
(resolution of, by microcolumn chromatog.)
RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)

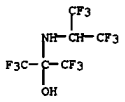


L10 ANSWER 82 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB The synthesis of a series of phosphinic acid dipeptide analogs, NH2CH(R1)PO(OH)CH2CH(R2)CO2H, related to D-Ala-D-Ala, is reported. The best of these compds. are potent, essentially irreversible inhibitors of D-Ala-D-Ala ligase, and their preferred stereochem. was shown by chiral synthesis of (1-S)-aminoethyl)(2R)-carboxy-1-n-propyl)phosphinic acid (I) and by x-ray crystallog. of its derivative benzyl [1(S)-[(benzyloxycarbonyl)amino]ethyl](2(R)-carbomethoxy-1-propyl)phosphinate, to correspond to the stereochem. configuration of D-Ala-D-Ala at both centers. A mechanism for the inhibition of D-Ala-D-Ala ligase by these compds. is proposed to involve an ATP-dependent formation of phosphorylated inhibitor within the enzyme's active site. The antibacterial activities of the compds. are modest although their spectra include both Gram-pos. and Gram-neg. susceptible organisms. The best antibacterial activity was shown by (1(S)-aminoethyl)[2-carboxy-2(R)-methylthio-1-ethyl]phosphinic acid, whose MICs range 4-128 mg/mL on 9 of 11 bacteria. Combination of an active phosphinic acid, I, with the alanine racemase inhibitor fluoro-D-alanine enhances the antibacterial spectrum of the latter on several strains of bacteria and inhibits fluoro-D-alanine's self-reversal, which normally occurs at concns. several fold higher than its MIC level. This inhibition of fluoro-D-alanine self-reversal is consistent with an involvement of D-Ala-D-Ala ligase inhibition in the antibacterial activity of these compds.
ACCESSION NUMBER: 1989:20972 CAPLUS
DOCUMENT NUMBER: 110:20972
TITLE: Phosphinic acid inhibitors of D-alanyl-D-alanine ligase
AUTHOR(S): Parsons, William H.; Patchett, Arthur A.; Bull, Herbert G.; Schoen, William R.; Taub, David; Davidson, Jacqueline; Combs, Patricia L.; Springer, James P.; Gadebusch, Hans; et al.
CORPORATE SOURCE: Merck Inst. Ther. Res., Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (1988), 31(9), 1772-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:20972
IT **35455-20-0**
RL: BIOL (Biological study)
(bactericidal activities of phosphinic acid alanylalanine ligase inhibitors combined with)
RN 35455-20-0 CAPLUS
CN D-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

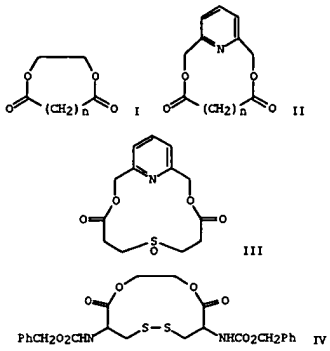


L10 ANSWER 83 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB Reaction of H2P[C(CF3)2OH] with HN:C(CF3)2 gave HP[C(CF3)2OH][C(CF3)2NH2] (I) which was also prepared by the reaction of H2P[C(CF3)2NH2] with (F3C)2CO. Silylation of HP[C(CF3)2OH]2 with Me3SiCl-(Me3Si)2NH gave HP[C(CF3)2OSiMe3][C(CF3)2OH] (II), whereas silylation of I gave HP[C(CF3)2OSiMe3][C(CF3)2NH2]. Silylation of II with same reagents gave HP[C(CF3)2OSiMe3]2 which was halogenated with N-halosuccinimide to give XP[C(CF3)2OSiMe3]2 (X = Cl, Br). 19F-19F homocorrelated 2D spectrum of I showed a long range 19F-19F couplings probably via a nonbond mechanism.
ACCESSION NUMBER: 1988:37948 CAPLUS
DOCUMENT NUMBER: 108:37948
TITLE: Bis[2,2,2-trifluoro-1-(trifluoromethyl)ethyl]phosphine
AUTHOR(S): Kischkel, Helmut; Francke, Rudolph; Roeschenthaler, Gerd Volker
CORPORATE SOURCE: Univ. Bremen, Bremen, 2800/33, Fed. Rep. Ger.
SOURCE: Revue de Chimie Minerale (1986), 23(45), 690-700
CODEN: RVCMA8; ISSN: 0035-1032
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 108:37948
IT **112313-46-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 112313-46-9 CAPLUS
CN 2-Propanol, 1,1,1,3,3,3-hexafluoro-2-[[2,2,2-trifluoro-1-(trifluoromethyl)ethyl]amino]- (9CI) (CA INDEX NAME)



IT **1619-92-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hexafluoroacetone)
RN 1619-92-7 CAPLUS
CN 2-Propanamine, 1,1,1,3,3,3-hexafluoro- (9CI) (CA INDEX NAME)

L10 ANSWER 84 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI

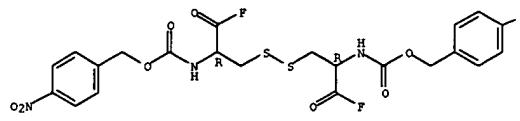


AB Intermol. condensation of (Ph3Sn0)2Q (Q = CH2CH2, 2,6-pyridinediyldioxy) with diacid difluorides (FCO)2Q1 [Q1 = (CH2)n (n = 3, 4, 6), CH(NHCO2CH2Ph)CH2CH2] gave microcyclic dilactones, e.g., I (n = 4, 6), II (m = 3, 6), including dilactones containing S, S2, and S(O) moieties, e.g., III, IV. Thus, Ph3SnOSnPh3 was treated with HOCH2CH2OH, then with FCO(CH2)4COF to give 35% I (n = 4). Chiral macrocyclic dilactones were prepared from optically active amino acids. In some cases, formation of dilactones was accompanied by formation of tetralactones and oligomeric lactones. Effects of dilution, temperature, and ring-size on the reaction were examined The binding abilities of the dilactones were determined
by pick rate extraction from H2O to CHCl3. In some cases, selective complexation of Ca2+ was observed
ACCESSION NUMBER: 1987:617502 CAPLUS
DOCUMENT NUMBER: 107:217502
TITLE: Synthesis of macrocyclic dilactones with the aid of organotin compounds. Application to sulfur macrocycles (sulfides, sulfoxides, disulfides). Selective complexation with calcium ion
AUTHOR(S): Picard, C.; Cazaux, L.; Tisnes, P.
CORPORATE SOURCE: Univ. Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron (1986), 42(13), 3503-19
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 107:217502
IT **95107-93-0P**

L10 ANSWER 84 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and condensation of, with triphenyltin deriv.)
RN 95107-93-0 CAPLUS
CN 2-Oxa-7,8-dithia-4,11-diazadodecan-12-oic acid, 5,10-bis(fluorocarbonyl)-1-(4-nitrophenyl)-3-oxo-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

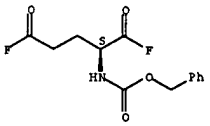


PAGE 1-B



IT **95107-91-8P 95107-92-9P 110270-46-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, with triphenyltin derivs.)
RN 95107-91-8 CAPLUS
CN Carbamic acid, [4-fluoro-1-(fluorocarbonyl)-4-oxobutyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

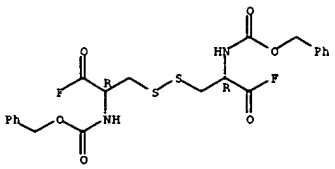
Absolute stereochemistry.



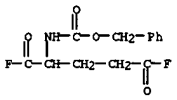
RN 95107-92-9 CAPLUS
CN 2-Oxa-7,8-dithia-4,11-diazadodecan-12-oic acid, 5,10-bis(fluorocarbonyl)-3-oxo-1-phenyl-, phenylmethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 84 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 110270-46-7 CAPLUS
CN Carbamic acid, [4-fluoro-1-(fluorocarbonyl)-4-oxobutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)



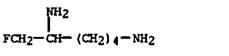
L10 ANSWER 85 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

AB Capillary gas chromatog. (GC) on chiral stationary phases, i.e., Chirasil-Val [L-valine-tert-(R)-α-butylamide] and XE-60-S-valine-(R)-α-phenylethylamide, has been applied to the resolution of various substituted analogs of putrescine as their N,N'-perfluoroacyl derivs. The influence of the nature of the substituent on the retention behavior and on the resolution of the enantiomers was studied. The results are discussed in terms of volatility and interaction with the chiral stationary phase. The 1,4-disubstituted putrescine analogs with 2 chiral centers were also clearly resolved into their corresponding stereoisomers. When the chain length between the 2 amino groups was increased, no clear resolution was obtained of the monosubstituted cadaverine analogs as their N,N'-perfluoroacyl derivs. However, resolution was obtained after derivatization of the cadaverine analogs with (-)-α-methoxy-α-trifluoromethylphenylacetyl chloride, followed by GC anal. on an achiral phase.

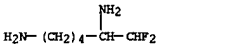
ACCESSION NUMBER: 1987:571733 CAPLUS
DOCUMENT NUMBER: 107:171733
TITLE: Separation of the enantiomers of substituted putrescine and cadaverine analogs by gas chromatography on chiral and achiral stationary phases
AUTHOR(S): Gaget, Christian; Wolf, Evelyne; Heintzelmann, Blanche; Wagner, Joseph
CORPORATE SOURCE: Strasbourg Cent., Merrell Dow Res. Inst., Strasbourg, 67084, Fr.
SOURCE: Journal of Chromatography (1987), 395, 597-608
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **110764-69-7 110764-70-0 110764-71-1**
RL: ANT (Analyte); ANST (Analytical study)
(separation of, by gas chromatog.)

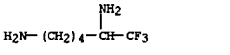
RN 110764-69-7 CAPLUS
CN 1,5-Hexanediamine, 6-fluoro- (9CI) (CA INDEX NAME)



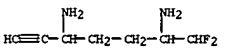
RN 110764-70-0 CAPLUS
CN 1,5-Hexanediamine, 6,6-difluoro- (9CI) (CA INDEX NAME)



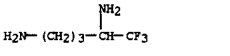
RN 110764-71-1 CAPLUS
CN 1,5-Hexanediamine, 6,6,6-trifluoro- (9CI) (CA INDEX NAME)



L10 ANSWER 85 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



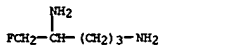
RN 110764-63-1 CAPLUS
CN 1,4-Pentanediamine, 5,5,5-trifluoro- (9CI) (CA INDEX NAME)



L10 ANSWER 85 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

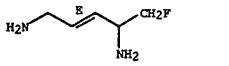
IT **69768-79-2 82006-58-4 86120-58-3**
**86559-36-6 86617-99-4 86634-46-0**
**110764-63-1**
RL: PROC (Process)
(separation of, by gas chromatog. as trifluoroacetyl derivative)

RN 69768-79-2 CAPLUS
CN 1,4-Pentanediamine, 5-fluoro- (9CI) (CA INDEX NAME)

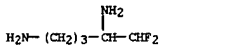


RN 82006-58-4 CAPLUS
CN 2-Pentene-1,4-diamine, 5-fluoro-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

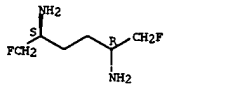


RN 86120-58-3 CAPLUS
CN 1,4-Pentanediamine, 5,5-difluoro- (9CI) (CA INDEX NAME)

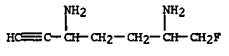


RN 86559-36-6 CAPLUS
CN 2,5-Hexanediamine, 1,6-difluoro-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 86617-99-4 CAPLUS
CN 6-Heptyne-2,5-diamine, 1-fluoro- (9CI) (CA INDEX NAME)



RN 86634-46-0 CAPLUS
CN 6-Heptyne-2,5-diamine, 1,1-difluoro- (9CI) (CA INDEX NAME)

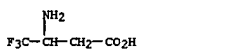
L10 ANSWER 86 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN

AB Gas chromatog. (GC) with a chiral stationary phase, Chirasil-Val, was used for separation of the enantiomers of several analogs of α- and β-alanine as their N-trifluoroacetyl iso-Pr esters. The same chiral phase GC procedure was applied to the enantiomeric separation of various substituted GABA analogs. Reversed-phase HPLC with the chiral Cu-L-proline complex allowed a clear resolution of all the α-amino acids in their underivatized forms. It yielded somewhat smaller separation coeffs. for the substituted β-alanines and no resolution for the GABA analogs. The influence of the nature of the amino acid, α, β, or γ, and the effects of the different substituents on the separation coeffs. obtained by GC and HPLC are discussed.

ACCESSION NUMBER: 1987:473572 CAPLUS
DOCUMENT NUMBER: 107:73572
TITLE: Chiral separation of enantiomers of substituted α- and β-alanine and γ-aminobutyric acid analogs by gas chromatography and high-performance liquid chromatography
AUTHOR(S): Wagner, J.; Wolf, E.; Heintzelmann, B.; Gaget, C.
CORPORATE SOURCE: Strasbourg Cent., Merrell Dow Res. Inst., Strasbourg, 67084, Fr.
SOURCE: Journal of Chromatography (1987), 392, 211-24
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

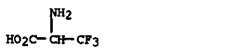
IT **584-20-3 16652-37-2 17463-43-3**
**35455-21-1 77162-46-0 77162-47-1**
**109537-89-5 109537-90-8 109584-01-2**
RL: PROC (Process)
(resolution of, by gas chromatog. and HPLC)

RN 584-20-3 CAPLUS
CN Butanoic acid, 3-amino-4,4,4-trifluoro- (9CI) (CA INDEX NAME)



RN 16652-37-2 CAPLUS
CN Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

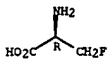
RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)



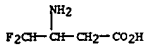
L10 ANSWER 86 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 35455-21-1 CAPLUS
CN L-Alanine, 3-fluoro- (9CI) (CA INDEX NAME)

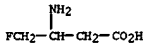
Absolute stereochemistry.



RN 77162-46-0 CAPLUS
CN Butanoic acid, 3-amino-4,4-difluoro- (9CI) (CA INDEX NAME)

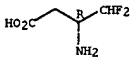


RN 77162-47-1 CAPLUS
CN Butanoic acid, 3-amino-4-fluoro- (9CI) (CA INDEX NAME)

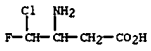


RN 109537-89-5 CAPLUS
CN Butanoic acid, 3-amino-4,4-difluoro-, (R)- (9CI) (CA INDEX NAME)

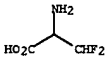
Absolute stereochemistry.



RN 109537-90-8 CAPLUS
CN Butanoic acid, 3-amino-4-chloro-4-fluoro- (9CI) (CA INDEX NAME)

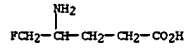


RN 109584-01-2 CAPLUS
CN Alanine, 3,3-difluoro- (9CI) (CA INDEX NAME)

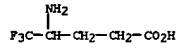


L10 ANSWER 86 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

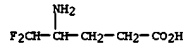
IT 70960-97-3 70961-08-9 78347-71-4
105457-53-2 105457-58-7
RL: PROC (Process)
(resolution of, by gas chromatog. as N-pentafluoropropionyl Et esters on Chirasil-Val, HPLC in relation to)
RN 70960-97-3 CAPLUS
CN Pentanoic acid, 4-amino-5-fluoro- (9CI) (CA INDEX NAME)



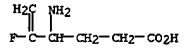
RN 70961-08-9 CAPLUS
CN Pentanoic acid, 4-amino-5,5,5-trifluoro- (9CI) (CA INDEX NAME)



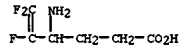
RN 78347-71-4 CAPLUS
CN Pentanoic acid, 4-amino-5,5-difluoro- (9CI) (CA INDEX NAME)



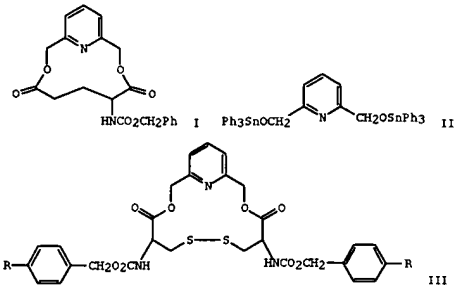
RN 105457-53-2 CAPLUS
CN 5-Hexenoic acid, 4-amino-5-fluoro- (9CI) (CA INDEX NAME)



RN 105457-58-7 CAPLUS
CN 5-Hexenoic acid, 4-amino-5,6,6-trifluoro- (9CI) (CA INDEX NAME)



L10 ANSWER 87 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI

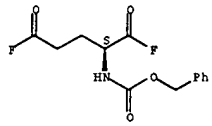


AB Glutamic acid macrocyclic dilactone I was prepared by cyclizing PhCH2O2CNHCH(COF)CH2CH2COF with tin compound II in benzene. Cystine macrocyclic dilactones III (R = H, NO2) were prepared similarly from the corresponding cystine difluorides and II. Complexing properties of I with cations were examined

ACCESSION NUMBER: 1985:113901 CAPLUS
DOCUMENT NUMBER: 102:113901
TITLE: Chiral macrocyclic dilactones derived from amino acids. Synthesis aided by organotin compounds; complexing properties
AUTHOR(S): Picard, C.; Cazaux, L.; Tisnes, P.
CORPORATE SOURCE: Lab. Synth. Physicochim. Org., Univ. Paul Sabatier, Toulouse, 31062, Fr.
SOURCE: Tetrahedron Letters (1984), 25(35), 3809-12
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: French
IT 95107-91-8P 95107-92-9P 95107-93-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with bis[(triphenylstannyloxy)methyl]pyridine, macrocyclic dilactone from)
RN 95107-91-8 CAPLUS
CN Carbamic acid, [4-fluoro-1-(fluorocarbonyl)-4-oxobutyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

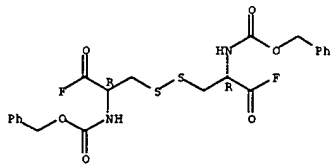
Absolute stereochemistry.

L10 ANSWER 87 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 95107-92-9 CAPLUS
CN 2-Oxa-7,8-dithia-4,11-diazadodecan-12-oic acid, 5,10-bis(fluorocarbonyl)-3-oxo-1-phenyl-, phenylmethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

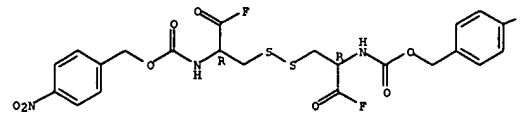
Absolute stereochemistry.



RN 95107-93-0 CAPLUS
CN 2-Oxa-7,8-dithia-4,11-diazadodecan-12-oic acid, 5,10-bis(fluorocarbonyl)-1-(4-nitrophenyl)-3-oxo-, (4-nitrophenyl)methyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

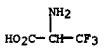
Absolute stereochemistry.

PAGE 1-A

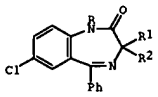


PAGE 1-B

L10 ANSWER 88 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB The separation of the enantiomers of underivatized amino acids can be easily realized by reversed-phase chromatog. with a chiral eluent. The eluent contains small concns. of Cu(II)-L-phenylalanine, N-methyl-, or N,N-dimethyl-L-phenylalanine complexes; the amino acids are separated via diastereomeric complexes by ligand-exchange chromatog. The retention of the amino acids is determined by the equilibrium of ligand-exchange and by hydrophobic interaction. The selectivity is strongly affected by pH value, the proportion of organic modifier, and the ionic strength. Rapid mass-transfer provides high column efficiency and, using short columns, chiral resolution can be achieved in less than 20 s. The application area is described which also involves the separation of α-hydroxy carboxylic acids.
ACCESSION NUMBER: 1985:109152 CAPLUS
DOCUMENT NUMBER: 102:109152
TITLE: Separation of underivatized amino acid enantiomers by means of a chiral solvent-generated phase
AUTHOR(S): Wernicke, Rainer
CORPORATE SOURCE: Chem. Reagents Div., E. Merck, Darmstadt, D-6100, Fed. Rep. Ger.
SOURCE: Journal of Chromatographic Science (1985), 23(1), 39-47
CODEN: JCHSBZ; ISSN: 0021-9665
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **17463-43-3**
RL: PROC (Process)
(resolution of, by ligand-exchange chromatog. with chiral solvent-generated phase)
RN 17463-43-3 CAPLUS
CN Alanine, 3,3,3-trifluoro- (9CI) (CA INDEX NAME)



L10 ANSWER 89 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
GI

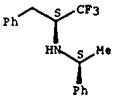


I

AB Alkylation of benzodiazepinones I (R = H, Me, CHMePh; R1 = R2 = H) gave I (R1 = CO2Et, Me, Et, CH2Ph, R2 = H), which underwent H-D exchange to give I (R2 = D). I (R = H, R1 = CO2Et, R2 = D) was reduced with NaAlEtZH2 to give I (R = H, R1 = CH2OH, R2 = D), which was silylated and fluorinated to give I (R = H, R1 = CH2F, R2 = D). Alkaline hydrolysis of the latter compound
gave (±)-HO2CCD(NH2)CH2F.
ACCESSION NUMBER: 1981:497753 CAPLUS
DOCUMENT NUMBER: 95:97753
TITLE: Chiral 1,4-benzodiazepin-2-one, template for enantioselective synthesis of α-amino acids and their α-deuterio congeners
AUTHOR(S): Decorte, Enio; Toso, Roberto; Sega, Alessandro; Sunjic, Vitomir; Ruzic-Toros, Ziva; Kojic-Prodic, Biserka; Bresciani-Pahor, Nevenka; Nardin, Giorgio; Randaccio, Lucio
CORPORATE SOURCE: CRC, Chem. Res. Co., Italy
SOURCE: Helvetica Chimica Acta (1981), 64(4), 1145-9
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:97753
IT **59189-03-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59189-03-6 CAPLUS
CN Alanine-2-d, 3-fluoro- (9CI) (CA INDEX NAME)

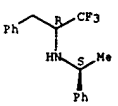
L10 ANSWER 90 OF 90 CAPLUS COPYRIGHT 2005 ACS on STN
AB (S)-(-)-PhCHMeNH2 with ketones PhCOCF3, PhCH2COCF3, or PhCO(CF2)2CF3 gave the chiral imines, which were reduced to the amines, e.g., with (MeOCH2CH2O)2AlH. Hydrogenolysis of chiral amine PhCH(CF3)NHCHMePh over Pd on charcoal gave (s)-(+)-PhCH(CF3)NH2 (I). The diastereoisomeric carbamates derived from I and chloroformates of (R)-(-)-menthol or (R)-(-)-2-octanol showed greater chromatog. separation and
an inverted elution order compared to nonfluorinated analogs.
ACCESSION NUMBER: 1977:452888 CAPLUS
DOCUMENT NUMBER: 87:52888
TITLE: Design of chiral derivatizing agents for the chromatographic resolution of optical isomers. Asymmetric synthesis of some chiral fluoroalkylated amines
AUTHOR(S): Pirkle, W. H.; Hauske, J. R.
CORPORATE SOURCE: Sch. Chem. Sci., Univ. Illinois, Urbana, IL, USA
SOURCE: Journal of Organic Chemistry (1977), 42(14), 2436-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **62198-03-2P 62198-04-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 62198-03-2 CAPLUS
CN Benzeneethanamine, N-(1-phenylethyl)-α-(trifluoromethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 62198-04-3 CAPLUS
CN Benzeneethanamine, N-(1-phenylethyl)-α-(trifluoromethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=>  logoff yh
'YH' IS NOT VALID HERE
For an explanation, enter "HELP LOGOFF".

=> logoff y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   211.63     676.38

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -29.93     -50.37

STN INTERNATIONAL LOGOFF AT 15:56:02 ON 21 MAY 2005
```